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STRUCTURE-BASED DRUG DESIGN FOR ULP1 PROTEASE SUBSTRATES

This application claims priority under 35 U.S.C. §119 from provisional patent application Serial No. 60/205,336, filed May 18, 2000; which is hereby incorporated by reference in its entirety.

FIELD OF THE INVENTION

The present invention relates to rational drug design of cysteine protease inhibitors based on the crystal structure of a Ulp1 protease trapped with its substrate in a covalent intermediate.

BACKGROUND OF THE INVENTION

Ubiquitin (Ub) and ubiquitin-like (Ubl) proteins modulate protein function in the cell through covalent modification of the target protein. Two proteins that have been identified as belonging to this family are ubiquitin and Small Ubiquitin-related Modifier (SUMO-1). The Ub/Ubl conjugated state of cellular proteins has been associated with several critical pathways, including cellular differation, apoptosis, the cell-cycle, and cellular responses to stress (Hershko and Ciehanover, 1998, Annu. Rev. Biochem., 67:425; Hochstrasser, 1998, Genes and Develop., 12:901; Laney and Hochstrasser, 1999; Cell, 97:427, Saitoh, *et al.*, 1997, TIBS, 22:374; Johnson and Hochstrasser, 1997, Trends. Cell. Biol., 7:408). Alterations in the regulation of the Ub/Ubl pathway has been implicated in several disease states, including tumorogenesis and acute promyelocytic leukemia (Hershko and Ciehanover, 1998, Annu. Rev. Biochem., 67:425; Kamitani *et al.*, 1998, J. Biol. Chem., 273:26675).

Ub and Ubl proteins are covalently attached to their cellular targets via a reversible amide linkage between a lysine ε-amino group on the target and the C-terminus of the Ub/Ubl

protein. The fate of the modified protein depends on if it is conjugated to ubiquitin or SUMO-1. Ubiquinated and poly-ubiquinated proteins are generally targeted to the 26S proteosome for degradation in cell-cycle dependent and cell-cycle independent pathways. Sumoylated protein targets appear to modulate the activity of the targeted system either directly or indirectly by altering cellular localization. Cellular pathways that appear to be modulated by the SUMO pathway include activation of RanGAP1, p53 transcriptional regulation, and Iκbα protection from ubiquitination (Matunis, *et al.*, 1996; J. Cell. Biol., 135:1457, Gostissa, *et al.*, 1999, EMBO J., 18:6462; Rodriguez, *et al.*, 1999, EMBO J., 18:6455, Desterro, *et al.*, 1998; Mol. Cell., 2:233). Ub/Ubl modifiers are generally deconjugated from their cellular targets by a class of cysteine proteases, known as deubiquinating (DUB) enzymes.

Studies in yeast show that Smt3, a yeast member of the Ubl protein family, conjugation and deconjugation to proteins appears critical to several yeast functions, including septin ring formation, chromosomal segregation, and progression of the cell cycle. Smt3 shares 47% sequence identity with mammalian SUMO-1 and 17% sequence identity with ubiquitin. Recently, studies showed the identification of a novel *Saccharomyces cerevisiae* gene product termed Ubl-specific protease 1 (Ulp1). In contrast to the ubiquitin DUB system, Ulp1 catalyzes Smt3 processing and Smt3-protein deconjugation.

There is a continuing need in the art to develop methods that enable one to evaluate interactions between proteases and their substrates. The development of an efficient method of trapping the protease and substrate in a complex, which would allow for the study of these interactions is needed. Such a method could allow for the development of compounds that could specifically interact with the amino acids necessary for protease function.

U.S. Patent No. 5,834,228 discloses the use of rational drug design for developing inhibitors of the apopain that will form non-covalent interactions with active site, as based on the crystal structure of the protease and substrate. The reference, however, does not indicate how to trap the protease and substrate in a reaction intermediate state or use this method for identifying compounds that produce covalent interactions with the protease. Thus, there is a need in the art to define active site structures of cystine proteases complexed with their substrates.

SUMMARY OF THE INVENTION

The present invention provides for a composition that is comprised of a polypeptide that comprises the catalytic domain of a SUMO protease and its substrate. In the composition, the SUMO protease is trapped in a deacylation intermediate complex with the substrate.

The invention further provides for a method of forming a complex between a polypeptide that comprises the catalytic domain of a protease with its substrate by (1) combining the protease and substrate in a molar ratio; (2) adding a reducing agent, which is capable of trapping a proteolytic deacylation intermediate complex of the protease and substrate, in an amount that is effective to trap the protease and substrate and (3) adjusting the pH of the mixture to about 7.0.

The present invention provides for polynucleotide sequence that encodes a mutant Ulp1. The mutant Ulp1 may contain an amino acid substitution at position 432, 448, 451 472, 474, 489, 490, 493, or 515. The invention also provides for vectors containing polynucleotide sequences of the mutant Ulp1, cells with the vectors containing the mutant Ulp1 polynucleotide sequences, and the mutant Ulp1 polypeptides.

The present invention also advantageously provides a method of identifying potential substrates of cystine proteases by rational drug design. The method is comprised of designing candidate substrates that form interactions with catalytic amino acids which are identified from computer modeling studies based on the crystal structure of the complex of the protease and substrate.

BRIEF DESCRIPTION OF DRAWINGS

Figure 1A and 1B. Stereo images of the Ulp1 active site in complex with Smt3. Hydrogen bonds are represented as black spheres. Cys580, His541, and Asp351 represent the catalytic triad in the protease fold.

DETAILED DESCRIPTION OF THE INVENTION

The present invention advantageously provides an isolated, preferably purified, trapped protease-substrate complex, preferably a cysteine protease. In particular, protease-

substrate complexes of the invention are those of the sumo pathway, involved in many important cellular processes.

The invention is based, in part, on trapping and crystallization of a Ulp1-Smt3 covalent complex, from which the Ulp1 crystal structure was obtained (coordinates are attached as Table 1 (after the specification and before the claims) and deposited in the Protein Data Bank with accession no. NC-001148). This crystal structure permits the rational drug design of Ulp1 and Ulp1 ortholog inhibitions, which function to promote ubiquitin and ubiquitin-like protein activities in cells.

General Definitions

As used herein, the term "isolated" means that the referenced material is removed from the environment in which it is normally found. Thus, an isolated biological material can be free of cellular components, *i.e.*, components of the cells in which the material is found or produced. In the case of nucleic acid molecules, an isolated nucleic acid includes a PCR product, an isolated mRNA, a cDNA, or a restriction fragment. In another embodiment, an isolated nucleic acid is preferably excised from the chromosome in which it may be found, and more preferably is no longer joined to non-regulatory, non-coding regions, or to other genes, located upstream or downstream of the gene contained by the isolated nucleic acid molecule when found in the chromosome. In yet another embodiment, the isolated nucleic acid lacks one or more introns. Isolated nucleic acid molecules include sequences inserted into plasmids, cosmids, artificial chromosomes, and the like. Thus, in a specific embodiment, a recombinant nucleic acid is an isolated nucleic acid. An isolated protein may be associated with other proteins or nucleic acids, or both, with which it associates in the cell, or with cellular membranes if it is a membrane-associated protein. An isolated organelle, cell, or tissue is removed from the anatomical site in which it is found in an organism. An isolated material may be, but need not be, purified.

The term "purified" as used herein refers to material that has been isolated under conditions that reduce or eliminate the presence of unrelated materials, *i.e.*, contaminants, including native materials from which the material is obtained. For example, a purified protein is preferably substantially free of other proteins or nucleic acids with which it is associated in a cell; a purified

nucleic acid molecule is preferably substantially free of proteins or other unrelated nucleic acid molecules with which it can be found within a cell. As used herein, the term "substantially free" is used operationally, in the context of analytical testing of the material. Preferably, purified material substantially free of contaminants is at least 50% pure; more preferably, at least 90% pure, and more preferably still at least 99% pure. Purity can be evaluated by chromatography, gel electrophoresis, immunoassay, composition analysis, biological assay, and other methods known in the art.

Methods for purification are well-known in the art. For example, nucleic acids can be purified by precipitation, chromatography (including preparative solid phase chromatography, oligonucleotide hybridization, and triple helix chromatography), ultracentrifugation, and other means. Polypeptides and proteins can be purified by various methods including, without limitation, preparative disc-gel electrophoresis, isoelectric focusing, HPLC, reversed-phase HPLC, gel filtration, ion exchange and partition chromatography, precipitation and salting-out chromatography, extraction, and countercurrent distribution. For some purposes, it is preferable to produce the polypeptide in a recombinant system in which the protein contains an additional sequence tag that facilitates purification, such as, but not limited to, a polyhistidine sequence, or a sequence that specifically binds to an antibody, such as FLAG and GST. The polypeptide can then be purified from a crude lysate of the host cell by chromatography on an appropriate solid-phase matrix. Alternatively, antibodies produced against the protein or against peptides derived therefrom can be used as purification reagents. Cells can be purified by various techniques, including centrifugation, matrix separation (*e.g.*, nylon wool separation), panning and other immunoselection techniques, depletion (*e.g.*, complement depletion of contaminating cells), and cell sorting (*e.g.*, fluorescence activated cell sorting [FACS]). Other purification methods are possible. A purified material may contain less than about 50%, preferably less than about 75%, and most preferably less than about 90%, of the cellular components with which it was originally associated. The "substantially pure" indicates the highest degree of purity which can be achieved using conventional purification techniques known in the art. In a specific embodiment, the term "about" or "approximately" means within 20%, preferably within 10%, and more preferably within 5% of a given value or range.

A "sample" as used herein refers to a biological material which can be tested for the presence of Ulp1 protein or *Ulp1* nucleic acids. Such samples can be obtained from animal subjects,

such as humans and non-human animals, and include tissue, biopsies, blood and blood products; plural effusions; cerebrospinal fluid (CSF); ascites fluid; and cell culture.

The term "about" or "approximately" means within an acceptable error range for a given measurement. In one aspect, the error range can be within 25% of a value, preferably within 10%, and more preferably within 5%. Alternatively, particularly in biological systems, an acceptable error is one order of magnitude, preferably 2-fold.

The use of italics indicates a nucleic acid molecule (*e.g.*, *Ulp1* cDNA, gene, etc.); normal text indicates the polypeptide or protein.

Cloning and Expression of mutant *Ulp1*

The present invention contemplates generation of a gene encoding wild-type or a mutant Ulp1, including a full length and any antigenic fragments thereof from any source, preferably human. It further contemplates detection of mutant Ulp1 protein for evaluation, diagnosis, or therapy.

In accordance with the present invention there may be employed conventional molecular biology, microbiology, and recombinant DNA techniques within the skill of the art. Such techniques are explained fully in the literature. See, *e.g.*, Sambrook, Fritsch & Maniatis, *Molecular Cloning: A Laboratory Manual,* Second Edition (1989) Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York (herein "Sambrook *et al.*, 1989"); *DNA Cloning: A Practical Approach,* Volumes I and II (D.N. Glover ed. 1985); *Oligonucleotide Synthesis* (M.J. Gait ed. 1984); *Nucleic Acid Hybridization* [B.D. Hames & S.J. Higgins eds. (1985)]; *Transcription And Translation* [B.D. Hames & S.J. Higgins, eds. (1984)]; *Animal Cell Culture* [R.I. Freshney, ed. (1986)]; *Immobilized Cells And Enzymes* [IRL Press, (1986)]; B.Perbal, *A Practical Guide To Molecular Cloning* (1984); F.M. Ausubel *et al.* (eds.), *Current Protocols in Molecular Biology*, John Wiley & Sons, Inc. (1994).

Molecular Biology - Definitions

"Amplification" of DNA as used herein denotes the use of polymerase chain reaction (PCR) to increase the concentration of a particular DNA sequence within a mixture of DNA sequences. For a description of PCR see Saiki *et al.*, Science, 239:487, 1988.

The polynucleotides encoding Ulp1 herein may be flanked by natural regulatory (expression control) sequences, or may be associated with heterologous sequences, including promoters, internal ribosome entry sites (IRES) and other ribosome binding site sequences, enhancers, response elements, suppressors, signal sequences, polyadenylation sequences, introns, 5'- and 3'- non-coding regions, and the like. The nucleic acids may also be modified by many means known in the art. Non-limiting examples of such modifications include methylation, "caps", substitution of one or more of the naturally occurring nucleotides with an analog, and internucleotide modifications such as, for example, those with uncharged linkages (*e.g.*, methyl phosphonates, phosphotriesters, phosphoroamidates, carbamates, etc.) and with charged linkages (*e.g.*, phosphorothioates, phosphorodithioates, etc.). Polynucleotides may contain one or more additional covalently linked moieties, such as, for example, proteins (*e.g.*, nucleases, toxins, antibodies, signal peptides, poly-L-lysine, etc.), intercalators (*e.g.*, acridine, psoralen, etc.), chelators (*e.g.*, metals, radioactive metals, iron, oxidative metals, etc.), and alkylators. The polynucleotides may be derivatized by formation of a methyl or ethyl phosphotriester or an alkyl phosphoramidate linkage. Furthermore, the polynucleotides herein may also be modified with a label capable of providing a detectable signal, either directly or indirectly. Exemplary labels include radioisotopes, fluorescent molecules, biotin, and the like.

The term "host cell" means any cell of any organism that is selected, modified, transformed, grown, or used or manipulated in any way, for the production of a substance by the cell, for example the expression by the cell of a gene, a DNA or RNA sequence, a protein or an enzyme. Host cells can further be used for screening or other assays, as described *infra*.

Proteins and enzymes are made in the host cell using instructions in DNA and RNA, according to the genetic code. Generally, a DNA sequence having instructions for a particular protein or enzyme is "transcribed" into a corresponding sequence of RNA. The RNA sequence in turn is "translated" into the sequence of amino acids which form the protein or enzyme. An "amino acid sequence" is any chain of two or more amino acids. Each amino acid is represented in DNA or RNA by one or more triplets of nucleotides. Each triplet forms a codon, corresponding to an amino acid. For example, the amino acid lysine (Lys) can be coded by the nucleotide triplet or codon AAA or by the codon AAG. (The genetic code has some redundancy, also called degeneracy,

meaning that most amino acids have more than one corresponding codon.) Because the nucleotides in DNA and RNA sequences are read in groups of three for protein production, it is important to begin reading the sequence at the correct amino acid, so that the correct triplets are read. The way that a nucleotide sequence is grouped into codons is called the "reading frame."

A "coding sequence" or a sequence "encoding" an expression product, such as a RNA, polypeptide, protein, or enzyme, is a nucleotide sequence that, when expressed, results in the production of that RNA, polypeptide, protein, or enzyme, *i.e.*, the nucleotide sequence encodes an amino acid sequence for that polypeptide, protein or enzyme. A coding sequence for a protein may include a start codon (usually ATG) and a stop codon.

A "promoter sequence" is a DNA regulatory region capable of binding RNA polymerase in a cell and initiating transcription of a downstream (3' direction) coding sequence. For purposes of defining the present invention, the promoter sequence is bounded at its 3' terminus by the transcription initiation site and extends upstream (5' direction) to include the minimum number of bases or elements necessary to initiate transcription at levels detectable above background. Within the promoter sequence will be found a transcription initiation site (conveniently defined for example, by mapping with nuclease S1), as well as protein binding domains (consensus sequences) responsible for the binding of RNA polymerase.

A coding sequence is "under the control" or "operatively associated with" of transcriptional and translational control sequences in a cell when RNA polymerase transcribes the coding sequence into mRNA, which is then trans-RNA spliced (if it contains introns) and translated into the protein encoded by the coding sequence.

The terms "express" and "expression" mean allowing or causing the information in a gene or DNA sequence to become manifest, for example producing a protein by activating the cellular functions involved in transcription and translation of a corresponding gene or DNA sequence. A DNA sequence is expressed in or by a cell to form an "expression product" such as a protein. The expression product itself, *e.g.* the resulting protein, may also be said to be "expressed" by the cell. An expression product can be characterized as intracellular, extracellular or secreted. The term "intracellular" means something that is inside a cell. The term "extracellular" means

something that is outside a cell. A substance is "secreted" by a cell if it appears in significant measure outside the cell, from somewhere on or inside the cell.

The term "transfection" means the introduction of a foreign nucleic acid into a cell. The term "transformation" means the introduction of a "foreign" (*i.e.* extrinsic or extracellular) gene, DNA or RNA sequence to a host cell, so that the host cell will express the introduced gene or sequence to produce a desired substance, typically a protein or enzyme coded by the introduced gene or sequence. The introduced gene or sequence may also be called a "cloned" or "foreign" gene or sequence, may include regulatory or control sequences, such as start, stop, promoter, signal, secretion, or other sequences used by a cell's genetic machinery. The gene or sequence may include nonfunctional sequences or sequences with no known function. A host cell that receives and expresses introduced DNA or RNA has been "transformed" and is a "transformant" or a "clone." The DNA or RNA introduced to a host cell can come from any source, including cells of the same genus or species as the host cell, or cells of a different genus or species.

The terms "vector", "cloning vector" and "expression vector" mean the vehicle by which a DNA or RNA sequence (*e.g.* a foreign gene) can be introduced into a host cell, so as to transform the host and promote expression (*e.g.* transcription and translation) of the introduced sequence. Vectors include plasmids, phages, viruses, etc.; they are discussed in greater detail below.

Vectors typically comprise the DNA of a transmissible agent, into which foreign DNA is inserted. A common way to insert one segment of DNA into another segment of DNA involves the use of enzymes called restriction enzymes that cleave DNA at specific sites (specific groups of nucleotides) called restriction sites. A "cassette" refers to a DNA coding sequence or segment of DNA that codes for an expression product that can be inserted into a vector at defined restriction sites. The cassette restriction sites are designed to ensure insertion of the cassette in the proper reading frame. Generally, foreign DNA is inserted at one or more restriction sites of the vector DNA, and then is carried by the vector into a host cell along with the transmissible vector DNA. A segment or sequence of DNA having inserted or added DNA, such as an expression vector, can also be called a "DNA construct." A common type of vector is a "plasmid", which generally is a self-contained molecule of double-stranded DNA, usually of bacterial origin, that can readily accept additional (foreign) DNA and which can readily introduced into a suitable host cell. A

plasmid vector often contains coding DNA and promoter DNA and has one or more restriction sites suitable for inserting foreign DNA. Coding DNA is a DNA sequence that encodes a particular amino acid sequence for a particular protein or enzyme. Promoter DNA is a DNA sequence which initiates, regulates, or otherwise mediates or controls the expression of the coding DNA. Promoter DNA and coding DNA may be from the same gene or from different genes, and may be from the same or different organisms. A large number of vectors, including plasmid and fungal vectors, have been described for replication and/or expression in a variety of eukaryotic and prokaryotic hosts. Non-limiting examples include pKK plasmids (Clonetech), pUC plasmids, pET plasmids (Novagen, Inc., Madison, WI), pRSET or pREP plasmids (Invitrogen, San Diego, CA), or pMAL plasmids (New England Biolabs, Beverly, MA), and many appropriate host cells, using methods disclosed or cited herein or otherwise known to those skilled in the relevant art. Recombinant cloning vectors will often include one or more replication systems for cloning or expression, one or more markers for selection in the host, *e.g.* antibiotic resistance, and one or more expression cassettes.

The term "expression system" means a host cell and compatible vector under suitable conditions, *e.g.* for the expression of a protein coded for by foreign DNA carried by the vector and introduced to the host cell. Common expression systems include *E. coli* host cells and plasmid vectors, insect host cells and *Baculovirus* vectors, and mammalian host cells and vectors.

The term "heterologous" refers to a combination of elements not naturally occurring. For example, heterologous DNA refers to DNA not naturally located in the cell, or in a chromosomal site of the cell. Preferably, the heterologous DNA includes a gene foreign to the cell. A heterologous expression regulatory element is a such an element operatively associated with a different gene than the one it is operatively associated with in nature. In the context of the present invention, a *Ulp1* gene is heterologous to the vector DNA in which it is inserted for cloning or expression, and it is heterologous to a host cell containing such a vector, in which it is expressed, *e.g.*, a yeast cell.

The terms "mutant" and "mutation" mean any detectable change in genetic material, *e.g.* DNA, or any process, mechanism, or result of such a change. This includes gene mutations, in which the structure (*e.g.* DNA sequence) of a gene is altered, any gene or DNA arising from any mutation process, and any expression product (*e.g.* protein or enzyme) expressed by a modified gene

or DNA sequence. The term "variant" may also be used to indicate a modified or altered gene, DNA sequence, enzyme, cell, etc., *i.e.*, any kind of mutant.

"Sequence-conservative variants" of a polynucleotide sequence are those in which a change of one or more nucleotides in a given codon position results in no alteration in the amino acid encoded at that position.

"Function-conservative variants" are those in which a given amino acid residue in a protein or enzyme has been changed without altering the overall conformation and function of the polypeptide, including, but not limited to, replacement of an amino acid with one having similar properties (such as, for example, polarity, hydrogen bonding potential, acidic, basic, hydrophobic, aromatic, and the like). Amino acids with similar properties are well known in the art. For example, arginine, histidine and lysine are hydrophilic-basic amino acids and may be interchangeable. Similarly, isoleucine, a hydrophobic amino acid, may be replaced with leucine, methionine or valine. Such changes are expected to have little or no effect on the apparent molecular weight or isoelectric point of the protein or polypeptide. Amino acids other than those indicated as conserved may differ in a protein or enzyme so that the percent protein or amino acid sequence similarity between any two proteins of similar function may vary and may be, for example, from 70% to 99% as determined according to an alignment scheme such as by the Cluster Method, wherein similarity is based on the MEGALIGN algorithm. A "function-conservative variant" also includes a polypeptide or enzyme which has at least 60 % amino acid identity as determined by BLAST or FASTA algorithms, preferably at least 75%, most preferably at least 85%, and even more preferably at least 90%, and which has the same or substantially similar properties or functions as the native or parent protein or enzyme to which it is compared.

As used herein, the term "homologous" in all its grammatical forms and spelling variations refers to the relationship between proteins that possess a "common evolutionary origin," including proteins from superfamilies (*e.g.*, the immunoglobulin superfamily) and homologous proteins from different species (*e.g.*, myosin light chain, etc.) (Reeck *et al.*, 1987, Cell 50:667). Such proteins (and their encoding genes) have sequence homology, as reflected by their sequence similarity, whether in terms of percent similarity or the presence of specific residues or motifs at conserved positions.

Accordingly, the term "sequence similarity" in all its grammatical forms refers to the degree of identity or correspondence between nucleic acid or amino acid sequences of proteins that may or may not share a common evolutionary origin (*see* Reeck *et al.*, *supra*). However, in common usage and in the instant application, the term "homologous," when modified with an adverb such as "highly," may refer to sequence similarity and may or may not relate to a common evolutionary origin.

In a specific embodiment, two DNA sequences are "substantially homologous" or "substantially similar" when at least about 80%, and most preferably at least about 90 or 95%) of the nucleotides match over the defined length of the DNA sequences, as determined by sequence comparison algorithms, such as BLAST, FASTA, DNA Strider, etc. An example of such a sequence is an allelic or species variant of the specific *Ulp1* genes of the invention. Sequences that are substantially homologous can be identified by comparing the sequences using standard software available in sequence data banks, or in a Southern hybridization experiment under, for example, stringent conditions as defined for that particular system.

Similarly, in a particular embodiment, two amino acid sequences are "substantially homologous" or "substantially similar" when greater than 80% of the amino acids are identical, or greater than about 90% are similar (functionally identical). Preferably, the similar or homologous sequences are identified by alignment using, for example, the GCG (Genetics Computer Group, Program Manual for the GCG Package, *Version 7*, Madison, Wisconsin) pileup program, or any of the programs described above (BLAST, FASTA, etc)

A nucleic acid molecule is "hybridizable" to another nucleic acid molecule, such as a cDNA, genomic DNA, or RNA, when a single stranded form of the nucleic acid molecule can anneal to the other nucleic acid molecule under the appropriate conditions of temperature and solution ionic strength (*see* Sambrook *et al.*, *supra*). The conditions of temperature and ionic strength determine the "stringency" of the hybridization. For preliminary screening for homologous nucleic acids, low stringency hybridization conditions, corresponding to a T_m (melting temperature) of 55°C, can be used, *e.g.*, 5x SSC, 0.1% SDS, 0.25% milk, and no formamide; or 30% formamide, 5x SSC, 0.5% SDS). Moderate stringency hybridization conditions correspond to a higher T_m, *e.g.*, 40% formamide, with 5x or 6x SCC. High stringency hybridization conditions correspond to the

highest T_m, *e.g.*, 50% formamide, 5x or 6x SCC. SCC is a 0.15M NaCl, 0.015M Na-citrate. Hybridization requires that the two nucleic acids contain complementary sequences, although depending on the stringency of the hybridization, mismatches between bases are possible. The appropriate stringency for hybridizing nucleic acids depends on the length of the nucleic acids and the degree of complementation, variables well known in the art. The greater the degree of similarity or homology between two nucleotide sequences, the greater the value of T_m for hybrids of nucleic acids having those sequences. The relative stability (corresponding to higher T_m) of nucleic acid hybridizations decreases in the following order: RNA:RNA, DNA:RNA, DNA:DNA. For hybrids of greater than 100 nucleotides in length, equations for calculating T_m have been derived (*see* Sambrook *et al.*, *supra*, 9.50-9.51). For hybridization with shorter nucleic acids, *i.e.*, oligonucleotides, the position of mismatches becomes more important, and the length of the oligonucleotide determines its specificity (*see* Sambrook *et al.*, *supra*, 11.7-11.8). A minimum length for a hybridizable nucleic acid is at least about 10 nucleotides; preferably at least about 15 nucleotides; and more preferably the length is at least about 20 nucleotides.

In a specific embodiment, the term "standard hybridization conditions" refers to a T_m of 55°C, and utilizes conditions as set forth above. In a preferred embodiment, the T_m is 60°C; in a more preferred embodiment, the T_m is 65°C. In a specific embodiment, "high stringency" refers to hybridization and/or washing conditions at 68°C in 0.2XSSC, at 42°C in 50% formamide, 4XSSC, or under conditions that afford levels of hybridization equivalent to those observed under either of these two conditions.

As used herein, the term "oligonucleotide" refers to a nucleic acid, generally of at least 10, preferably at least 15, and more preferably at least 20 nucleotides, preferably no more than 100 nucleotides, that is hybridizable to a genomic DNA molecule, a cDNA molecule, or an mRNA molecule encoding a gene, mRNA, cDNA, or other nucleic acid of interest. Oligonucleotides can be labeled, *e.g.*, with ^{32}P-nucleotides or nucleotides to which a label, such as biotin, has been covalently conjugated. In one embodiment, a labeled oligonucleotide can be used as a probe to detect the presence of a nucleic acid. In another embodiment, oligonucleotides (one or both of which may be labeled) can be used as PCR primers, either for cloning full length or a fragment of Ulp1, or to detect the presence of nucleic acids encoding Ulp1. In a further embodiment, an

oligonucleotide of the invention can form a triple helix with a Ulp1 DNA molecule. Generally, oligonucleotides are prepared synthetically, preferably on a nucleic acid synthesizer. Accordingly, oligonucleotides can be prepared with non-naturally occurring phosphoester analog bonds, such as thioester bonds, etc.

Ulp1 Nucleic Acids

A gene encoding mutant Ulp1, whether genomic DNA or cDNA, can be isolated from any source, particularly from a human cDNA or genomic library. Methods for obtaining *Ulp1* gene are well known in the art, as described above (*see, e.g.*, Sambrook *et al.*, 1989, *supra*). The DNA may be obtained by standard procedures known in the art from cloned DNA (*e.g.*, a DNA "library"), and preferably is obtained from a cDNA library prepared from tissues with high level expression of the protein, by chemical synthesis, by cDNA cloning, or by the cloning of genomic DNA, or fragments thereof, purified from the desired cell (See, for example, Sambrook *et al.*, 1989, *supra*; Glover, D.M. (ed.), 1985, DNA Cloning: A Practical Approach, MRL Press, Ltd., Oxford, U.K. Vol. I, II). Clones derived from genomic DNA may contain regulatory and intron DNA regions in addition to coding regions; clones derived from cDNA will not contain intron sequences. Whatever the source, the gene should be molecularly cloned into a suitable vector for propagation of the gene. Identification of the specific DNA fragment containing the desired *Ulp1* gene may be accomplished in a number of ways. For example, a portion of an *Ulp1* gene exemplified *infra* can be purified and labeled to prepare a labeled probe, and the generated DNA may be screened by nucleic acid hybridization to the labeled probe (Benton and Davis, Science 196:180, 1977; Grunstein and Hogness, Proc. Natl. Acad. Sci. U.S.A. 72:3961, 1975). Those DNA fragments with substantial homology to the probe, such as an allelic variant from another individual, will hybridize.

Further selection can be carried out on the basis of the properties of the gene, *e.g.*, if the gene encodes a protein product having the isoelectric, electrophoretic, amino acid composition, partial or complete amino acid sequence, antibody binding activity, or ligand binding profile of *Ulp1* protein as disclosed herein. Thus, the presence of the gene may be detected by assays based on the physical, chemical, immunological, or functional properties of its expressed product.

Other DNA sequences which encode substantially the same amino acid sequence as an *Ulp1* gene may be used in the practice of the present invention. These include but are not limited to allelic variants, species variants, sequence conservative variants, and functional variants.

Amino acid substitutions may also be introduced to substitute an amino acid with a particularly preferable property. For example, a Cys may be introduced a potential site for disulfide bridges with another Cys.

The genes encoding *Ulp1* derivatives and analogs of the invention can be produced by various methods known in the art. The manipulations which result in their production can occur at the gene or protein level. For example, the cloned *Ulp1* gene sequence can be modified by any of numerous strategies known in the art (Sambrook *et al.*, 1989, *supra*). The sequence can be cleaved at appropriate sites with restriction endonuclease(s), followed by further enzymatic modification if desired, isolated, and ligated *in vitro*. In the production of the gene encoding a derivative or analog of *Ulp1*, care should be taken to ensure that the modified gene remains within the same translational reading frame as the *Ulp1* gene, uninterrupted by translational stop signals, in the gene region where the desired activity is encoded.

Additionally, the *Ulp1* encoding nucleic acid sequence can be mutated *in vitro* or *in vivo*, to create and/or destroy translation, initiation, and/or termination sequences, or to create variations in coding regions and/or form new restriction endonuclease sites or destroy preexisting ones, to facilitate further *in vitro* modification. Such modifications can be made to introduce restriction sites and facilitate cloning the *Ulp1* gene into an expression vector. Any technique for mutagenesis known in the art can be used, including but not limited to, *in vitro* site-directed mutagenesis (Hutchinson, C., *et al.*, J. Biol. Chem. 253:6551, 1978; Zoller and Smith, DNA 3:479-488, 1984; Oliphant *et al.*, Gene 44:177, 1986; Hutchinson *et al.*, Proc. Natl. Acad. Sci. U.S.A. 83:710, 1986), use of TAB™ linkers (Pharmacia), etc. PCR techniques are preferred for site directed mutagenesis (see Higuchi, 1989, "Using PCR to Engineer DNA", in *PCR Technology: Principles and Applications for DNA Amplification*, H. Erlich, ed., Stockton Press, Chapter 6, pp. 61-70).

The identified and isolated gene can then be inserted into an appropriate cloning vector. A large number of vector-host systems known in the art may be used. Possible vectors include, but are not limited to, plasmids or modified viruses, but the vector system must be

compatible with the host cell used. Examples of vectors include, but are not limited to, *E. coli*, bacteriophages such as lambda derivatives, or plasmids such as pBR322 derivatives or pUC plasmid derivatives, *e.g.*, pGEX vectors, pmal-c, pFLAG, etc. The insertion into a cloning vector can, for example, be accomplished by ligating the DNA fragment into a cloning vector which has complementary cohesive termini. However, if the complementary restriction sites used to fragment the DNA are not present in the cloning vector, the ends of the DNA molecules may be enzymatically modified. Alternatively, any site desired may be produced by ligating nucleotide sequences (linkers) onto the DNA termini; these ligated linkers may comprise specific chemically synthesized oligonucleotides encoding restriction endonuclease recognition sequences.

Recombinant molecules can be introduced into host cells via transformation, transfection, infection, electroporation, etc., so that many copies of the gene sequence are generated. Preferably, the cloned gene is contained on a shuttle vector plasmid, which provides for expansion in a cloning cell, *e.g.*, *E. coli*, and facile purification for subsequent insertion into an appropriate expression cell line, if such is desired. For example, a shuttle vector, which is a vector that can replicate in more than one type of organism, can be prepared for replication in both *E. coli* and *Saccharomyces cerevisiae* by linking sequences from an *E. coli* plasmid with sequences form the yeast 2μ plasmid.

Expression of Ulp1 Polypeptides

The nucleotide sequence coding for Ulp1, or antigenic fragment, derivative or analog thereof, or a functionally active derivative, including a chimeric protein, thereof, can be inserted into an appropriate expression vector, *i.e.*, a vector which contains the necessary elements for the transcription and translation of the inserted protein-coding sequence. Thus, a nucleic acid encoding Ulp1 of the invention can be operationally associated with a promoter in an expression vector of the invention. Both cDNA and genomic sequences can be cloned and expressed under control of such regulatory sequences. Such vectors can be used to express functional or functionally inactivated Ulp1 polypeptides.

The necessary transcriptional and translational signals can be provided on a recombinant expression vector, or they may be supplied by the native gene encoding Ulp1 and/or its flanking regions.

Potential host-vector systems include but are not limited to mammalian cell systems transfected with expression plasmids or infected with virus (*e.g.*, vaccinia virus, adenovirus, adeno-associated virus, herpes virus, etc.); insect cell systems infected with virus (*e.g.*, baculovirus); microorganisms such as yeast containing yeast vectors; or bacteria transformed with bacteriophage, DNA, plasmid DNA, or cosmid DNA. The expression elements of vectors vary in their strengths and specificities. Depending on the host-vector system utilized, any one of a number of suitable transcription and translation elements may be used.

Expression of Ulp1 protein may be controlled by any promoter/enhancer element known in the art, but these regulatory elements must be functional in the host selected for expression. Promoters which may be used to control Ulp1 gene expression include, but are not limited to, cytomegalovirus (CMV) promoter, the SV40 early promoter region (Benoist and Chambon, 1981, Nature 290:304-310), the promoter contained in the 3' long terminal repeat of Rous sarcoma virus (Yamamoto, *et al.*, Cell 22:787-797, 1980), the herpes thymidine kinase promoter (Wagner *et al.*, Proc. Natl. Acad. Sci. U.S.A. 78:1441-1445, 1981), the regulatory sequences of the metallothionein gene (Brinster *et al.*, Nature 296:39-42, 1982); prokaryotic expression vectors such as the β-lactamase promoter (Villa-Komaroff, *et al.*, Proc. Natl. Acad. Sci. U.S.A. 75:3727-3731, 1978), or the *tac* promoter (DeBoer, *et al.*, Proc. Natl. Acad. Sci. U.S.A. 80:21-25, 1983); see also "Useful proteins from recombinant bacteria" in Scientific American, 242:74-94, 1980; promoter elements from yeast or other fungi such as the Gal 4 promoter, the ADC (alcohol dehydrogenase) promoter, PGK (phosphoglycerol kinase) promoter, alkaline phosphatase promoter; and transcriptional control regions that exhibit tissue specificity, particularly endothelial cell-specific promoters.

Soluble forms of the protein can be obtained by collecting culture fluid, or solubilizing inclusion bodies, *e.g.*, by treatment with detergent, and if desired sonication or other mechanical processes, as described above. The solubilized or soluble protein can be isolated using various techniques, such as polyacrylamide gel electrophoresis (PAGE), isoelectric focusing, 2-dimensional gel electrophoresis, chromatography (*e.g.*, ion exchange, affinity, immunoaffinity,

and sizing column chromatography), centrifugation, differential solubility, immunoprecipitation, or by any other standard technique for the purification of proteins.

Vectors

A wide variety of host/expression vector combinations may be employed in expressing the DNA sequences of this invention. Useful expression vectors, for example, may consist of segments of chromosomal, non-chromosomal and synthetic DNA sequences. Suitable vectors include derivatives of SV40 and known bacterial plasmids, *e.g.*, *E. coli* plasmids col El, pCR1, pBR322, pMal-C2, pET, pGEX (Smith *et al.*, Gene 67:31-40, 1988), pMB9 and their derivatives, plasmids such as RP4; phage DNAS, *e.g.*, the numerous derivatives of phage l, *e.g.*, NM989, and other phage DNA, *e.g.*, M13 and filamentous single stranded phage DNA; yeast plasmids such as the 2μ plasmid or derivatives thereof; vectors useful in eukaryotic cells, such as vectors useful in insect or mammalian cells; vectors derived from combinations of plasmids and phage DNAs, such as plasmids that have been modified to employ phage DNA or other expression control sequences; and the like.

Preferred vectors for introducing Ulp1 coding sequences into mammalian or insect cells are viral vectors, such as lentiviruses, retroviruses, herpes viruses, adenoviruses, adeno-associated viruses, vaccinia virus, baculovirus, and other recombinant viruses with desirable cellular tropism. Thus, a gene encoding a functional or mutant Ulp1 protein or polypeptide domain fragment thereof can be introduced using a viral vector or through direct introduction of DNA.

Viral vectors commonly used for targeting procedures are DNA-based vectors and retroviral vectors. Methods for constructing and using viral vectors are known in the art (*see, e.g.*, Miller and Rosman, BioTechniques, 7:980-990, 1992). Preferably, the viral vectors are replication defective, that is, they are unable to replicate autonomously in the target cell. In general, the genome of the replication defective viral vectors which are used within the scope of the present invention lack at least one region which is necessary for the replication of the virus in the infected cell. These regions can either be eliminated (in whole or in part), be rendered non-functional by any technique known to a person skilled in the art. These techniques include the total removal, substitution (by other sequences, in particular by the inserted nucleic acid), partial deletion or addition of one or more

bases to an essential (for replication) region. Such techniques may be performed *in vitro* (on the isolated DNA) or *in situ*, using the techniques of genetic manipulation or by treatment with mutagenic agents. Preferably, the replication defective virus retains the sequences of its genome which are necessary for encapsidating the viral particles.

DNA viral vectors include an attenuated or defective DNA virus, such as but not limited to herpes simplex virus (HSV), papillomavirus, Epstein Barr virus (EBV), adenovirus, adeno-associated virus (AAV), and the like. Defective viruses, which entirely or almost entirely lack viral genes, are preferred. Defective virus is not infective after introduction into a cell. Use of defective viral vectors allows for administration to cells in a specific, localized area, without concern that the vector can infect other cells. Thus, a specific tissue can be specifically targeted. Examples of particular vectors include, but are not limited to, a defective herpes virus 1 (HSV1) vector (Kaplitt *et al.*, Molec. Cell. Neurosci. 2:320-330, 1991), defective herpes virus vector lacking a glyco-protein L gene (Patent Publication RD 371005 A), or other defective herpes virus vectors (International Patent Publication No. WO 94/21807, published September 29, 1994; International Patent Publication No. WO 92/05263, published April 2, 1994); an attenuated adenovirus vector, such as the vector described by Stratford-Perricaudet *et al.* (J. Clin. Invest. 90:626-630, 1992; see also La Salle *et al.*, Science 259:988-990, 1993); and a defective adeno-associated virus vector (Samulski *et al.*, J. Virol. 61:3096-3101, 1987; Samulski *et al.*, J. Virol. 63:3822-3828, 1989; Lebkowski *et al.*, Mol. Cell. Biol. 8:3988-3996, 1988).

Various companies produce viral vectors commercially, including but by no means limited to Avigen, Inc. (Alameda, CA; AAV vectors), Cell Genesys (Foster City, CA; retroviral, adenoviral, AAV vectors, and lentiviral vectors), Clontech (retroviral and baculoviral vectors), Genovo, Inc. (Sharon Hill, PA; adenoviral and AAV vectors), Genvec (adenoviral vectors), IntroGene (Leiden, Netherlands; adenoviral vectors), Molecular Medicine (retroviral, adenoviral, AAV, and herpes viral vectors), Norgen (adenoviral vectors), Oxford BioMedica (Oxford, United Kingdom; lentiviral vectors), and Transgene (Strasbourg, France; adenoviral, vaccinia, retroviral, and lentiviral vectors).

In another embodiment, the vector can be introduced by lipofection, as naked DNA, or with other transfection facilitating agents (peptides, polymers, etc.). Synthetic cationic lipids can

be used to prepare liposomes for *in vivo* transfection of a gene encoding a marker (Felgner, et. al., Proc. Natl. Acad. Sci. U.S.A. 84:7413-7417, 1987; Felgner and Ringold, Science 337:387-388, 1989; see Mackey, *et al.*, Proc. Natl. Acad. Sci. U.S.A. 85:8027-8031, 1988; Ulmer, *et al.*, Science 259:1745-1748, 1993). Useful lipid compounds and compositions for transfer of nucleic acids are described in International Patent Publications WO95/18863 and WO96/17823, and in U.S. Patent No. 5,459,127. Lipids may be chemically coupled to other molecules for the purpose of targeting (see Mackey, *et al.*, *supra*). Targeted peptides, *e.g.*, hormones or neurotransmitters, and proteins such as antibodies, or non-peptide molecules could be coupled to liposomes chemically.

Other molecules are also useful for facilitating transfection of a nucleic acid, such as a cationic oligopeptide (*e.g.*, International Patent Publication WO95/21931), peptides derived from DNA binding proteins (*e.g.*, International Patent Publication WO96/25508), or a cationic polymer (*e.g.*, International Patent Publication WO95/21931).

Alternatively, non-viral DNA vectors can be introduced into the desired host cells by methods known in the art, *e.g.*, electroporation, microinjection, cell fusion, DEAE dextran, calcium phosphate precipitation, use of a gene gun (ballistic transfection; see, *e.g.*, U.S. Pat. No. 5,204,253, U.S. Pat. No. 5,853,663, U.S. Pat. No. 5,885,795, and U.S. Pat. No. 5,702,384 and see Sanford, TIB-TECH, 6:299-302, 1988; Fynan *et al.*, Proc. Natl. Acad. Sci. U.S.A., 90:11478-11482, 1993; and Yang *et al.*, Proc. Natl. Acad. Sci. U.S.A., 87:1568-9572, 1990), or use of a DNA vector transporter (see, *e.g.*, Wu, *et al.*, J. Biol. Chem. 267:963-967, 1992; Wu and Wu, J. Biol. Chem. 263:14621-14624, 1988; Hartmut, *et al.*, Canadian Patent Application No. 2,012,311, filed March 15, 1990; Williams, *et al.*, Proc. Natl. Acad. Sci. USA 88:2726-2730, 1991). Receptor-mediated DNA delivery approaches can also be used (Curiel, *et al.*, Hum. Gene Ther. 3:147-154, 1992; Wu and Wu, J. Biol. Chem. 262:4429-4432, 1987).

Protease-Substrate Complex Formation

The present invention describes a composition comprising a polypeptide of a SUMO protease catalytic domain in a trapped proteolytic deacylation intermediate complex with its substrate. The composition may then be treated with methods known in the art to produce a crystalline structure of the complex. The present invention contemplates characterization of the structure of any protease that produces deacylation intermediates upon interaction with a substrate, particularly any cysteine protease, *e.g.*, by trapping the protease-substrate covalent intermediate. Specifically, the present invention contemplates a composition where the SUMO protease is Ulp1. Ulp1 may be derived from various sources, including, but not limited to, mammal, yeast, insects, and plants. In one preferred embodiment, the Ulp1 is derived from mammal, specifically human. The composition may include any substrate of Ulp1, such as SUMO and Smt3. In a specific embodiment, the substrate is Smt3.

The complexed molecules in the composition are preferably obtained in a crystalline structure. The complexed molecules may be formed into a crystalline structure using techniques that are well known in the art, where the crystallizing conditions are modified and optimized for crystal formation of specific proteases and their substrate. Alternatively, other spectroscopic techniques for structure evaluation, such as nuclear magnetic resonance, Raman spectroscopy, circular dichroism, and neutron diffraction can be used to study trapped protease-substrate complexes.

The coordinates of atoms and structure of the protease and substrate in the crystal structure may be defined using any method and computational method needed. For example, if the protease and substrate complex are in a liquid form, then nuclear magnetic resonance can be used to determine the coordinates and structure of the complex. For complexes that are in a crystalline structure x-ray crystallography may be used to elucidate the structure.

The invention also describes a method of preparatively trapping and purifying large amounts of the proteolytic deacylation intermediate using a reducing agent. The method of trapping the proteolytic deacylation intermediate involves (a) combining the protease and substrate in a molar ratio, (b) adding a reducing agent that is capable of trapping the substrate in an intermediate state with the protease, and (c) then adjusting the pH of the solution to about 7.0. The invention allows for performing steps (a) and (b) in any order or simultaneously. In a

specific embodiment the protease is a SUMO protease, and more specifically the SUMO protease is the catalytic domain of Ulp1. Ulp1 may be derived from various sources, including, but not limited to, mammal, yeast, insects, and plants. In one preferred embodiment, the Ulp1 is derived from mammal, specifically human. The complex includes any substrate of Ulp1, such as SUMO and Smt3. In a specific embodiment, the substrate is Smt3.

The pH of the solution may be adjusted to about 7.0 by various methods known in the art, such as adding the required amount of an acid or base to the solution to adjust the pH to about 7.0. Other methods that may be used to adjust the pH of a solution, as appropriate for the system, include, but not limited to, chromatography and dialysis. In one embodiment of the invention, the pH of the solution is adjusted by dialysis. The protease-substrate complex may then be isolated from the solution after the pH is adjusted by dialysis. The protease-substrate complex may be isolated from the solution using any methods known in the art, including high performance liquid chromatography, size exclusion chromatography, dialysis, fast protein liquid chromatography, and crystallization. Other method of isolating the complex may be used, depending on the protease and substrate.

The molar ratio of protease to substrate may encompass any ratio where the concentration of substrate is in excess to insure that the protease may form a complex with it. Theoretically, the substrate may be in infinite excess to the protease, however that would lead to significant waste of substrate that remains uncomplexed to the protease. In the present invention the molar ratio of the protease to substrate ranges from 1:1 to 1:5. More preferred, the Ulp1 and Smt3 are in a 1:3 molar ratio.

The protease and substrate are trapped in a deacylation complex by addition of a reducing agent in an amount that is effective to trap the proteins. An effective amount of reducing agent is defined as the amount needed to trap an isolatable amount of the complex in the solution. Any reducing agent is contemplated by the present invention. However, several reducing agents, such as lithium aluminum hydride, could reduce other portions of the protease and substrate in the complex. In one specific embodiment the reducing agent is sodium borohydride.

Screening and Chemistry

According to the present invention, the structure of a Ulp1-Smt3 complex, or other trapped protease-substrate complexes, are useful to identify drugs that are effective in treating disorders associated with Ub/Ubl pathway, including tumorogenesis and acute promyelocytic leukemia.

Rational Drug Design

The invention also defines a method of identifying novel substrates for cysteine proteases by using rational drug design methods. The invention allows for designing substrates that would interact with amino acids in the protease catalytic site as defined by computer molecular modeling methods based on the crystal structure of the protease and other substrates. A substrate may include a competitive inhibitor, analog of the native substrate, or a suicide inhibitor. The designed substrates would be designed so that they interact with amino acid residues that are defined to be (i) necessary for interaction with a substrate and (ii) protease activity.

The present invention contemplates evaluating potential compounds for covalent and non-covalent interactions between the protease and substrate. Computer modeling methods that may be used to evaluate these interactions include, but are not limited to, SYBYL and Monte Carlo computer programs. The present invention contemplates computer algorithms that evaluate bonded and non-bonded interactions between the protease and the substrate. Bonded interactions that may be evaluated include, but are not limited to, bond stretching, rotational strain, and torsional strain. Non-bonded interactions that may be evaluated include van Der Waals forces, hydrogen bonds and dipole-dipole interaction.

In particular, identification of putative Ulp binding compounds provides for development of screening assays, particularly for high throughput screening of molecules that up- or down-regulate the activity of Ulp1, *e.g.*, by permitting expression of Ulp1 in quantities greater than can be isolated from natural sources, or in indicator cells that are specially engineered to indicate the activity of Ulp1 expressed after transfection or transformation of the cells.

Any screening technique known in the art can be used to screen for Ulp1 agonists or antagonists. The present invention contemplates screens for small molecule ligands or ligand analogs and mimics, as well as screens for natural ligands that bind to and agonize or antagonize

Ulp1 expression activity *in vivo*. For example, natural products libraries can be screened using assays of the invention for molecules that agonize or antagonize Ulp1 expression or activity.

Another approach uses recombinant bacteriophage to produce large libraries. Using the "phage method" (Scott and Smith, Science 249:386-390, 1990; Cwirla, *et al.*, Proc. Natl. Acad. Sci., 87:6378-6382, 1990; Devlin *et al.*, Science, 49:404-406, 1990), very large libraries can be constructed (10^6-10^8 chemical entities). A second approach uses primarily chemical methods, of which the Geysen method (Geysen *et al.*, Molecular Immunology 23:709-715, 1986; Geysen *et al.* J. Immunologic Method 102:259-274, 1987; and the method of Fodor *et al.* (Science 251:767-773, 1991) are examples. Furka *et al.* (14th International Congress of Biochemistry, Volume #5, Abstract FR:013, 1988; Furka, Int. J. Peptide Protein Res. 37:487-493, 1991), Houghton (U.S. Patent No. 4,631,211, issued December 1986) and Rutter *et al.* (U.S. Patent No. 5,010,175, issued April 23, 1991) describe methods to produce a mixture of peptides that can be tested as agonists or antagonists.

In another aspect, synthetic libraries (Needels *et al.*, Proc. Natl. Acad. Sci. USA 90:10700-4, 1993; Ohlmeyer *et al.*, Proc. Natl. Acad. Sci. USA 90:10922-10926, 1993; Lam *et al.*, International Patent Publication No. WO 92/00252; Kocis *et al.*, International Patent Publication No. WO 9428028) and the like can be used to screen for Ulp1 ligands according to the present invention.

Test compounds are screened from large libraries of synthetic or natural compounds. Numerous means are currently used for random and directed synthesis of saccharide, peptide, and nucleic acid based compounds. Synthetic compound libraries are commercially available from Maybridge Chemical Co. (Trevillet, Cornwall, UK), Comgenex (Princeton, NJ), Brandon Associates (Merrimack, NH), and Microsource (New Milford, CT). A rare chemical library is available from Aldrich (Milwaukee, WI). Alternatively, libraries of natural compounds in the form of bacterial, fungal, plant and animal extracts are available from *e.g.* Pan Laboratories (Bothell, WA) or MycoSearch (NC), or are readily producible. Additionally, natural and synthetically produced libraries and compounds are readily modified through conventional chemical, physical, and biochemical means (Blondelle *et al.*, Tib Tech, 14:60, 1996).

Knowledge of the crystal structure of Ulp1, particularly when trapped with a substrate, can provide an initial clue as the inhibitors or antagonists of the protein. Moreover, based

on sequence and enzymatic activity similarities of Ulp1 to other cysteine proteases, particularly cell-cycle associated cysteine proteases, the crystal structure of Ulp1 permits development of classes of cysteine protease inhibitors. Identification and screening of antagonists is further facilitated by determining structural features of the protein, *e.g.*, using X-ray crystallography, neutron diffraction, nuclear magnetic resonance spectrometry, and other techniques for structure determination. These techniques provide for the rational design or identification of agonists and antagonists.

In vivo *screening methods*

Intact cells or whole animals expressing a gene encoding Ulp1 can be used in screening methods to identify candidate drugs.

In one series of embodiments, a permanent cell line is established. Alternatively, cells (including without limitation mammalian, insect, yeast, or bacterial cells) are transiently programmed to express an *Ulp1* gene by introduction of appropriate DNA or mRNA. Identification of candidate compounds can be achieved using any suitable assay, including without limitation (i) assays that measure selective binding of test compounds to Ulp1 (ii) assays that measure the ability of a test compound to modify (*i.e.*, inhibit or enhance) a measurable activity or function of Ulp1 and (iii) assays that measure the ability of a compound to modify (*i.e.*, inhibit or enhance) the transcriptional activity of sequences derived from the promoter (*i.e.*, regulatory) regions the Ulp1 gene.

High-Throughput Screen

Agents according to the invention may be identified by screening in high-throughput assays, including without limitation cell-based or cell-free assays. It will be appreciated by those skilled in the art that different types of assays can be used to detect different types of agents. Several methods of automated assays have been developed in recent years so as to permit screening of tens of thousands of compounds in a short period of time. Such high-throughput screening methods are particularly preferred. The use of high-throughput screening assays to test for agents is greatly facilitated by the availability of large amounts of purified polypeptides, as provided by the invention.

EXAMPLES

The present invention will be better understood by reference to the following Examples, which are provided as exemplary of the invention, and not by way of limitation.

Materials and Methods

Protein purification

A Ulp1 amino acid fragment, from amino acids 403-621 (Ulp1(403-621)) , was amplified by polymerase chain reaction. The PCR fragment was digested with Nhe1 and Xho1 restriction endonucleases and then ligated into a pET-28b vector (Novagen). *E. coli* BL21 (DE3)pLysS bacterial cells were transformed with Ulp1(403-621). Cells were grown at 37° C for 20-24 hours. Cell cultures then were grown at 37° C in superbroth, containing 50 mg/ml kanamycin and 25 mg/ml chloamphenicol, by fermentation. When the A_{600} of the culture reached about 2.0 the culture was cooled to 30° C, adjusted to 1.0 mM IPTG, and fermented for about 4 hours at 30° C. Remaining steps were performed at 4° C. The culture was centrifuged and the cell pellet was resuspended in 200 mL lysis buffer (50 mM Tris-HCl, 0.15 mM NaCl, 20% (w/v) sucrose; pH = 8.0) and sonicated. Insoluble material was removed by centrifugation and the soluble fraction was placed over 10 mL of Ni-NTA-agarose resin (Qiagen) and washed with buffer A (50 mM Tris-HCl, 0.5 M NaCl, 20 mM imidazole). The protein was eluted from the resin with a gradient (20-300 mM imidazole) in buffer A. Peak fractions of His-tagged Ulp1(403-621)p were pooled and dialyzed against 50 mM Tris-HCl (pH=8.0) containing 200 mM NaCl, 2 mM β-mercaptoethanol, and 100 units bovine thrombin (Sigma) for about 20-24 hours.

A Smt3 PCR fragment (Smt3(13-101)p) was digested with Nco1 and Xho1 restriction endonucleases and then ligated into a pET-28b vector. *E. coli* BL21 (DE3)pLysS bacterial cells were transformed with Smt3(13-101)p. Expression and purification of the protein was performed following the same protocol as described for Ulp1(403-621)p, with the exception that the protein was dialyzed against 50 mM Tris-HCl (pH=8.0) containing 200 mM NaCl.

Sumo (??-101)p was prepared in a similar manner to that described for Smt3(13-101)p.

Selenomethionyl-containing Ulp1(403-621) was expressed in DL41 cells (methionine auxotrophe) that contained the bacteriophage T7 polymerase (Hendrickson *et al.*, EMBO J., 1990, 9:1665-1672).

The Smt3-GFPuv fusion protein was constructed by ligating SMT3 into the pGFPuv vector (Clontech). Smt3-GFPuv was overexpressed in JM109 *E. coli* strain. Purification was attained by standard chromatographic techniques and included passes over size exclusion, anion-exchange resins, and finally, application to a MonoQ column (Pharmacia). The Smt3-GFP moiety was followed during purification by analyzing fluorescence over a standard UV transilluminator.

His6-ubiquitin-Smt3-HA was expressed from pQE30 (Li and Hochstrasser) in JM109 *E. coli*. The histidine-tagged fusion protein (His6-ubiquitin-Smt3-HA) was placed over Ni-agarose resin, washed and eluted as previously described. The pooled fractions were then placed onto a gel filtration column (Superdex 75 prep-grade) for size exclusion. These fractions were pooled and placed onto a MonoQ column (Pharmacia) and eluted with a 0.02-1M gradient of NaCl. Smt3-GFP, Sumo-His, and His6-ubiquitin-Smt3-HA were concentrated to ~10 mg/ml and frozen at -80° C.

Proteolysis assays

Proteolysis assays were prepared by incubating a solution at about 37° C that contained about 1.0 mg/ml substrate and about 10^{-3}-10^{-6} mg/ml Ulp1(403-621)p in buffer containing 20mM Tris-HCl (pH = 8.0) and 150mM NaCl. The Smt3-GFP reaction was subsequently analyzed by native-gel electrophoresis. The reactions containing Sumo-His and His6-ubiquitin-Smt3-HA were analyzed by SDS-PAGE.

Synthesis of covalent adduct between Ulp1(403-621)p and Smt3(13-101)p

Ulp1(403-621)p and Smt3(13-101)p were placed in a beaker at a 1:3 molar ratio with stirring. Then 5 aliquots of sodium borohydride were stirred into the beaker over 30 minutes to a final concentration of 50 mM. The mixture was dialyzed against 20 mM Tris-HCl (pH=8.0) containing 20 mM NaCl at 4° C. The dialyzed solution was then loaded onto a Mono-Q column (Qiagen). The Ulp1(403-621)p -Smt3(13-101)p complex was eluted from the column with 0.02-0.5 M NaCl gradient. Fractions were analyzed by native gel electrophoresis. Ulp1(403-621)p -Smt3(13-

101)p was purified further by size exclusion chromatography on a Superdex75 prep-grade column (Pharmacia). Fractions were pooled, concentrated to about 3.5 mg/mL, and stored in 20 mM Tris-HCl containing 50 mM NaCl at -80° C.

Crystallization and data collection

Crystals were grown at 21° C by the hanging drop vapor diffusion method. Ulp1(403-621)p -Smt3(13-101)p complex was mixed with an equal volume of reservoir buffer containing 0.1 M MES (pH=6.5), 10% (w/v) polyethylene glycol 20000, and 3% (w/v) 1,6-hexandiol. Crystals were grown over several days to a size of 0.05x0.1x0.3 mm. Crystals were stabilized in reservoir solution for heavy atoms soaks and pre-incubated in reservoir solution plus 17% ethylene glycol. X-ray data used to collect native and heavy atom sets were collected using crystals at a laboratory copper Kα source (Rigaku RU200) equipped with a confocal optics and a Raxis-IV imaging plate detector system. The high-resolution native data set and a four-wavelength MAD data set were collected at the National Synchrotron Light Source (Brookhaven, NY) at beamline X4A on an ADSC Quantum-4 detector. Data were processed using DENZO and SCALEPACK. Ulp1(403-621)p -Smt3(13-101)p were crystallized in space group P21212 (a=125.8 Å, b=53.4 Å, c=54.3 Å, α=β=γ=90°).

Structure determination and refinement

2.6 Å electron density maps for the Ulp1(403-621)p -Smt3(13-101)p complex were initially derived using multiple isomorphous replacement (MIR) methods and solvent flattening (DM). Mercury sites were identified using Patterson methods and placed into MLPHARE for phase refinement. An initial trace into these maps was accomplished using the program O and the model was not refined. A selenomethionyl-derived Ulp1 (403-625)p and native Smt3(11-97)p crystal was subjected to a four-wavelength MAD experiment (Hendrickson, *et al.*, EMBO J., 1991, 9:1665-1672). The 1.8 Å MAD data was input into the program SOLVE (Terwilliger and Berendzen, Acta Crystallogr, 1999, D55:849-861). Six selenium sites were located and used to generate 1.8 Å phases. Solvent flattening was performed using the program DM (Cowtan, Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography, 1994, 31:34-38). The initial model derived from the MIR

electron density was placed into the MAD electron density maps for manual building. Refinement was accomplished using the programs REFMAC (Murshudov *et al.*, Acta. Crystallogr., 1997, A50:157-163) and wARP/ARP (Lamzin and Wilson, Acta. Crystallogr., 1993, D49:129-149) for automated building and placement of waters. The model underwent three rounds of refinement at 1.8 Å with manual rebuilding between each round. Refinement was extended to 1.6 Å for another round. The current model contains 735 waters and 303 amino acids (Rfree=25.3, R=17.9) and has excellent geometry; 92.9% of residues are in the most favored region of the Ramachandran plot with none occurring in disallowed regions. The model contained all 219 amino acid residues of Ulp1(403-621)p plus two additional N-terminal amino acids that correspond to residues left behind after thrombin cleavage of the N-terminally HIS-tagged protein. Ulp1p Arg422 did not have adequate density to model its side chain. The model for Smt3(13-98)p contains 79 of the possible 87 amino acid residues. Electron density for N-terminal Smt3 residues 12 through 19 could not be observed and were left out of the model.

09305424.030504

Yeast plasmids and strains

Standard techniques were used to grow and maintain yeast strains (Guthrie and Fink, Methods Enzymol., 1991; 194). Yeast strain W303-1A (MATa *ura3-1 ade2-1 trp1-1 his3, -1115, leu2-3, -112 can1-100*) was used to generate a Ulp1 null strain by one-step gene replacement procedure (Rothstein, Methods Enzymol., 1991; 194:281-301). The resulting strain was termed Ulp1Δ strain W303ULP1 (MATa *ura3-1 ade2-1 trp1-1 his3, -1115, leu2-3, -112 can1-100, Ulp1::LEU2*, pSE360-ULP1). *In vivo* complementation analysis was conducted using plasmid shaffle technique (Boeke *et al.*, Methods Enzymol., 1987; 154,164). W303ULP1 was transformed with pSE358 plasmid containing either wildtype or mutant Ulp1 under Ulp1 natural promoter. Yeast cells were streaked onto agar plates that lack tryptophan and incubated at about 30° C until yeast colonies were visible. Colonies were then restreaked onto agar plates containing and 5-fluoro-orotic acid to induce the loss of pSE360-ULP1.

Glacatose inducible expression

Wildtype or deletion mutant Ulp1 fragments were amplified by PCR. The fragments were digested with EcoR1 and BamH1 restriction endonucleases and ligated into PYX133 (*CEN TRP1* GAL promoter; Ingenius). W303-1A was transformed with the plasmid. Yeast strains were grown on plates lacking tryptophan, to select for cells that contain the plasmid of interest, at about 30° C. Positive yeast colonies were then streaked onto SD(-Trp) agar plates, containing 2% (w/v) raffinose, with and without 0.01% (w/v) galactose. Cells were incubated at 30° C until a color change in the yeast colonies was observed.

Point mutations were introduced to subcloned fragments using QuikChange Site-Directed Mutagenesis Kit (Qiagen).

Results

Ulp1(403-621)p displayed full catalytic activity in cleavage reactions with human SUMO-1 and yeast Smt3 to produce their respective mature protein forms (data not shown). Ulp1(403-621)p also showed full catalytic activity in deconjugation reactions with Smt3-GFPuv and His6-ubiquitin-Smt3-HA (data not shown), suggesting that the C-terminal fragment of Ulp1 (Ulp1(403-621)p) is able to (i) deconjugate large proteins and (ii) produce the mature forms of Smt3 and SUMO.

The secondary structure of Ulp1(403-621)p includes 7α helices and 7β strands. Ulp1(403-621)p exhibits structural similarities to other papain-like cysteine proteases in the active site, which includes the central α helix, 3β strands, and the catalytic triad (Cys-His-Glu/Asp) (Figure 1).

The Ulp1(403-621)p-Smt3(13-98)p structure is currently refined to 1.6 angstroms and includes all 219 amino acid residues of Ulp1(403-621)p and 79 of the possible 87 amino acid residues of Smt3(13-98)p. Coordinates of the Ulp1(403-621)p-Smt3(13-98)p structure are shown in Table 1 (present before the claims). The interaction between Ulp1 and Smt3 is described below in the context of six conserved Ulp1 motifs.

The interactions of motif 1 of Ulp1 with Smt3 include side-chain to main-chain hydrogen bonding, Van der Waals (VDW) contacts, and one salt bridge between Arg438 of Ulp1 and the Glu94 of Smt3.

Motif 2 of Ulp1 is involved in the recognition of residues at the C terminus of Smt3, including VDW contacts with the Gly-Gly motif of Smt3 by Trp448. Motif 2 also contributes (i) 3 hydrogen bonds to the main-chain of Smt3 strand 5 and (ii) 2 acidic residues (Glu455 and Asp451) that participate in salt-bridging interactions with 2 Smt3 basic residues (Arg64 and Arg71).

Motif 3 of Ulp1 provides direct hydrogen bonds to the main-chain of Smt3, Gly69, by a conserved Asn472. Hydrogen bonds are also made between Ser473 and Thr477 to an invariant Smt3 residue Gln95 in strand 5. VDW contacts in the Smt3-Ulp1 interface is contributed by Phe474.

Motif 4 of Ulp1 contains salt bridging moieties (Arg489 and Arg493) that make contact with two acidic residues in Smt3 (Asp68 and Asp82). Positions 489 and 493 also produce hydrogen bonds through water to make interactions with Asp87 in Smt3. Motif 4 contributes VDW contacts in the Ulp1-Smt3 interface through Trp490.

Motif 5 of Ulp1 contains His514, which is the general base of the catalytic triad. Motif 5 also participates in several interactions with the C-terminal tail of Smt3. Motif 5 contains Asn509 and Gln512, which participate in hydrogen bonds with main-chain atoms of Smt3 residues 94 and 96. The carbonyl of Ser513 is involved in a main-chain to main-chain hydrogen bond with Smt3 Gly98.

Motif 6 of Ulp1 contains active site amino acid residues Cys580 and Gln574, which are involved in the function of the protein.

* * *

The present invention is not to be limited in scope by the specific embodiments described herein. Indeed, various modifications of the invention in addition to those described herein will become apparent to those skilled in the art from the foregoing description and the accompanying figures. Such modifications are intended to fall within the scope of the appended claims.

It is further to be understood that values are approximate, and are provided for description.

Patents, patent applications, publications, procedures, and the like are cited

throughout this application, the disclosures of which are incorporated herein by reference in their entireties.

05650647 = 05/31/01

TABLE 1

```
HEADER    HYDROLASE                                17-APR-00   1EUV
TITLE     X-RAY STRUCTURE OF THE C-TERMINAL ULP1 PROTEASE DOMAIN IN
TITLE    2 COMPLEX WITH SMT3, THE YEAST ORTHOLOG OF SUMO.
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: ULP1 PROTEASE;
COMPND   3 CHAIN: A;
COMPND   4 FRAGMENT: C-TERMINAL PROTEASE DOMAIN;
COMPND   5 ENGINEERED: YES;
COMPND   6 MOL_ID: 2;
COMPND   7 MOLECULE: UBITQUTIN-LIKE PROTEIN SMT3;
COMPND   8 CHAIN: B;
COMPND   9 FRAGMENT: SMT3 RESIDUES 13-98;
COMPND  10 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: SACCHAROMYCES CEREVISIAE;
SOURCE   3 ORGANISM_COMMON: YEAST;
SOURCE   4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE   5 EXPRESSION_SYSTEM_COMMON: BACTERIA;
SOURCE   6 EXPRESSION_SYSTEM_PLASMID: PET28B;
SOURCE   7 MOL_ID: 2;
SOURCE   8 ORGANISM_SCIENTIFIC: SACCHAROMYCES CEREVISIAE;
SOURCE   9 ORGANISM_COMMON: YEAST;
SOURCE  10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE  11 EXPRESSION_SYSTEM_COMMON: BACTERIA;
SOURCE  12 EXPRESSION_SYSTEM_PLASMID: PET28B
KEYWDS    SUMO HYDROLASE, UBIQUITIN-LIKE PROTEASE 1, SMT3 HYDROLASE
KEYWDS   2 DESUMOYLATING ENZYME, CYSTEINE PROTEASE, SUMO PROCESSING
KEYWDS   3 ENZYME, SMT3 PROCESSING ENZYME, NABH4, THIOHEMIACETAL,
KEYWDS   4 COVALENT PROTEASE ADDUCT
EXPDTA    X-RAY DIFFRACTION
AUTHOR    E.MOSSESSOVA,C.D.LIMA
REVDAT   1   07-JUN-00 1EUV    0
JRNL        AUTH   E.MOSSESSOVA,C.D.LIMA
JRNL        TITL   ULP1-SUMO CRYSTAL STRUCTURE AND GENETIC ANALYSIS
JRNL        TITL 2 REVEAL CONSERVED INTERACTIONS AND A REGULATORY
JRNL        TITL 3 ELEMENT ESSENTIAL FOR CELL GROWTH IN YEAST
JRNL        REF    MOL. CELL                     V.   5   865 2000
JRNL        REFN   ASTM MOCEFL  US ISSN 1097-2765
REMARK   1
REMARK   1 REFERENCE 1
REMARK   1  AUTH   S.J.LI,M.HOCHSTRASSER
REMARK   1  TITL   A NEW PROTEASE REQUIRED FOR CELL-CYCLE PROGRESSION
REMARK   1  TITL 2 IN YEAST.
REMARK   1  REF    NATURE                        V. 398   246 1999
REMARK   1  REFN   ASTM NATUAS  UK ISSN 0028-0836
REMARK   2
REMARK   2 RESOLUTION. 1.6 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.60
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 25.0
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 1.000
REMARK   3   COMPLETENESS FOR RANGE        (%) : 96.6
REMARK   3   NUMBER OF REFLECTIONS             : 47560
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
```

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REMARK   3   CROSS-VALIDATION METHOD          : NULL
REMARK   3   FREE R VALUE TEST SET SELECTION  : 5% OF THE OBSERVED
REMARK   3                                      DATA
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.193
REMARK   3   R VALUE           (WORKING SET) : 0.190
REMARK   3   FREE R VALUE                    : 0.251
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : NULL
REMARK   3   FREE R VALUE TEST SET COUNT      : 2378
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 2417
REMARK   3   NUCLEIC ACID ATOMS       : 0
REMARK   3   HETEROGEN ATOMS          : 0
REMARK   3   SOLVENT ATOMS            : 432
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : 20.69
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : NULL
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) : NULL
REMARK   3    B22 (A**2) : NULL
REMARK   3    B33 (A**2) : NULL
REMARK   3    B12 (A**2) : NULL
REMARK   3    B13 (A**2) : NULL
REMARK   3    B23 (A**2) : NULL
REMARK   3
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                                (A): NULL
REMARK   3   ESU BASED ON FREE R VALUE                           (A): NULL
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                     (A): NULL
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): NULL
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   DISTANCE RESTRAINTS.                        RMS    SIGMA
REMARK   3    BOND LENGTH                      (A) : 0.013 ; NULL
REMARK   3    ANGLE DISTANCE                   (A) : 1.600 ; NULL
REMARK   3    INTRAPLANAR 1-4 DISTANCE         (A) : NULL  ; NULL
REMARK   3    H-BOND OR METAL COORDINATION     (A) : NULL  ; NULL
REMARK   3
REMARK   3   PLANE RESTRAINT                   (A) : NULL  ; NULL
REMARK   3   CHIRAL-CENTER RESTRAINT       (A**3) : NULL  ; NULL
REMARK   3
REMARK   3   NON-BONDED CONTACT RESTRAINTS.
REMARK   3    SINGLE TORSION                   (A) : NULL  ; NULL
REMARK   3    MULTIPLE TORSION                 (A) : NULL  ; NULL
REMARK   3    H-BOND (X...Y)                   (A) : NULL  ; NULL
REMARK   3    H-BOND (X-H...Y)                 (A) : NULL  ; NULL
REMARK   3
REMARK   3   CONFORMATIONAL TORSION ANGLE RESTRAINTS.
REMARK   3    SPECIFIED                  (DEGREES) : NULL  ; NULL
REMARK   3    PLANAR                     (DEGREES) : NULL  ; NULL
REMARK   3    STAGGERED                  (DEGREES) : NULL  ; NULL
REMARK   3    TRANSVERSE                 (DEGREES) : NULL  ; NULL
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.    RMS    SIGMA
REMARK   3   MAIN-CHAIN BOND              (A**2) : NULL  ; NULL
REMARK   3   MAIN-CHAIN ANGLE             (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN BOND              (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN ANGLE             (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: USED A -LOGLIKELIHOOD RESIDUAL
REMARK   3  DERIVED FROM RICE DISTRIBUTION FOR CENTRIC AND ACENTRIC
REMARK   3  CASES OF FS SPARSE MATRIX PROCEDURE WITH ANISOTROPIC B-
REMARK   3  FACTOR REFINEMENT.
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REMARK   4
REMARK   4 1EUV COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK   6
REMARK   6 COVALENT ADDUCT FORMED BETWEEN THE PROTEOLYTIC
REMARK   6 ACTIVE SITE THIOL AND THE C-TERMINAL GLYCINE OF
REMARK   6 SMT3 USING THE REDUCING AGENT NABH4.
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 20-APR-2000
REMARK 100 THE RCSB ID CODE IS RCSB010911.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : 21-OCT-1999
REMARK 200  TEMPERATURE           (KELVIN) : 100.0
REMARK 200  PH                             : 6.50
REMARK 200  NUMBER OF CRYSTALS USED        : 1
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : Y
REMARK 200  RADIATION SOURCE               : NSLS
REMARK 200  BEAMLINE                       : X4A
REMARK 200  X-RAY GENERATOR MODEL          : NULL
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M
REMARK 200  WAVELENGTH OR RANGE        (A) : 0.9791
REMARK 200  MONOCHROMATOR                  : NULL
REMARK 200  OPTICS                         : NULL
REMARK 200
REMARK 200  DETECTOR TYPE                  : CCD
REMARK 200  DETECTOR MANUFACTURER          : ADSC QUANTUM 4
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200  DATA SCALING SOFTWARE          : SCALEPACK
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 47875
REMARK 200  RESOLUTION RANGE HIGH      (A) : 1.600
REMARK 200  RESOLUTION RANGE LOW       (A) : 25.000
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : 0.000
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : 96.6
REMARK 200  DATA REDUNDANCY                : 9.400
REMARK 200  R MERGE                    (I) : 0.04300
REMARK 200  R SYM                      (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : 16.4000
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 1.60
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 1.66
REMARK 200  COMPLETENESS FOR SHELL     (%) : 86.0
REMARK 200  DATA REDUNDANCY IN SHELL       : 4.30
REMARK 200  R MERGE FOR SHELL          (I) : 0.29000
REMARK 200  R SYM FOR SHELL            (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR SHELL         : NULL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: NULL
REMARK 200 SOFTWARE USED: SHARP
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): NULL
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 0.1M MES PH6.5, 10% W/V
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REMARK 280  POLYETHYLENE GLYCOL 20000, 3% W/V 1,6-HEXANDIOL
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 2
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
REMARK 290       2555   -X,-Y,Z
REMARK 290       3555   1/2-X,1/2+Y,-Z
REMARK 290       4555   1/2+X,1/2-Y,-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   3 -1.000000  0.000000  0.000000       62.88700
REMARK 290   SMTRY2   3  0.000000  1.000000  0.000000       26.58350
REMARK 290   SMTRY3   3  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   4  1.000000  0.000000  0.000000       62.88700                REMARK
290   SMTRY2   4  0.000000 -1.000000  0.000000       26.58350
REMARK 290   SMTRY3   4  0.000000  0.000000 -1.000000        0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465     GLU B    13
REMARK 465     VAL B    14
REMARK 465     LYS B    15                                                    REMARK 465
   PRO B    16
REMARK 465     GLU B    17
REMARK 465     VAL B    18
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REMARK 465     LYS B    19
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS(M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470   M RES CSSEQI  ATOMS
REMARK 470     PRO B  20    CB    CG    CD
REMARK 470     GLU B  21    CB    CG    CD    OE1   OE2
REMARK 470     LYS B  54    CG    CD    CE    NZ
REMARK 470     GLU B  59    CG    CD    OE1   OE2
REMARK 470     ASP B  75    CB    CG    OD1   OD2
REMARK 470     GLU B  84    CG    CD    OE1   OE2
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500  ATM1  RES C  SSEQI   ATM2  RES C  SSEQI
REMARK 500   NE   ARG A   422     O    HOH     377              1.12
REMARK 500   CD   ARG A   422     O    HOH     377              2.02            REMARK
500   O    HOH     272     NE   ARG A   422              2.14
REMARK 500   CZ   ARG A   422     O    HOH     377              2.17
REMARK 500   O    HOH     457     O    HOH     718              2.17            REMARK
500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS
REMARK 500
REMARK 500 THE FOLLOWING ATOMS THAT ARE RELATED BY CRYSTALLOGRAPHIC
REMARK 500 SYMMETRY ARE IN CLOSE CONTACT.  AN ATOM LOCATED WITHIN 0.15
REMARK 500 ANGSTROMS OF A SYMMETRY RELATED ATOM IS ASSUMED TO BE ON A
REMARK 500 SPECIAL POSITION AND IS, THEREFORE, LISTED IN REMARK 375
REMARK 500 INSTEAD OF REMARK 500.  ATOMS WITH NON-BLANK ALTERNATE
REMARK 500 LOCATION INDICATORS ARE NOT INCLUDED IN THE CALCULATIONS.
REMARK 500
REMARK 500 DISTANCE CUTOFF:
REMARK 500 2.2 ANGSTROMS FOR CONTACTS NOT INVOLVING HYDROGEN ATOMS
REMARK 500 1.6 ANGSTROMS FOR CONTACTS INVOLVING HYDROGEN ATOMS
REMARK 500
REMARK 500  ATM1  RES C  SSEQI   ATM2  RES C  SSEQI  SSYMOP   DISTANCE
REMARK 500   O    HOH     419     O    HOH       4     3558     1.28
REMARK 500   O    HOH     426     O    HOH       4     3558     1.62
REMARK 500   O    HOH      61     O    HOH     473     3558     1.68
REMARK 500   O    HOH     578     O    HOH      49     3548     2.07
REMARK 500   O    HOH     578     O    HOH      21     3548     2.18
REMARK 500   O    HOH      24     O    HOH     473     3558     2.18
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE  REMARK 500 THAN 6*RMSD
(M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,2(A3,1X,A1,I4,A1,1X,A4,3X),F6.3)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1   RES CSSEQI ATM2   DEVIATION
REMARK 500    ARG A 422   CB    ARG A 422   CA    -0.335
REMARK 500    GLY B  98   O     GLY B  98   C      0.125
```

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REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1   ATM2   ATM3
REMARK 500    ARG A 422   CB  -  CA  -  C   ANGL. DEV. = 21.6 DEGREES
REMARK 500    GLU A 423   CB  -  CG  -  CD  ANGL. DEV. = 27.4 DEGREES
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: TORSION ANGLES
REMARK 500
REMARK 500 TORSION ANGLES OUTSIDE THE EXPECTED RAMACHANDRAN REGIONS:
REMARK 500 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 500 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT:(10X,I3,1X,A3,1X,A1,I4,A1,4X,F7.2,3X,F7.2)
REMARK 500
REMARK 500  M RES CSSEQI         PSI       PHI
REMARK 500    GLU A 423      112.62    151.65
REMARK 525
REMARK 525 SOLVENT
REMARK 525 THE FOLLOWING SOLVENT MOLECULES LIE FARTHER THAN EXPECTED
REMARK 525 FROM THE PROTEIN OR NUCLEIC ACID MOLECULE AND MAY BE
REMARK 525 ASSOCIATED WITH A SYMMETRY RELATED MOLECULE (M=MODEL     REMARK 525 NUMBER;
RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE  REMARK 525 NUMBER; I=INSERTION CODE):

REMARK 525
REMARK 525  M RES CSSEQI
REMARK 525  0 HOH   322        DISTANCE =  6.11 ANGSTROMS
REMARK 525  0 HOH   420        DISTANCE =  6.85 ANGSTROMS
REMARK 525  0 HOH   457        DISTANCE =  7.05 ANGSTROMS
REMARK 525  0 HOH   544        DISTANCE =  7.02 ANGSTROMS
REMARK 525  0 HOH   627        DISTANCE =  7.46 ANGSTROMS
REMARK 525  0 HOH   673        DISTANCE =  8.63 ANGSTROMS
REMARK 525  0 HOH   718        DISTANCE =  5.47 ANGSTROMS
REMARK 525  0 HOH   746        DISTANCE =  5.09 ANGSTROMS
REMARK 999
REMARK 999 SEQUENCE
REMARK 999 RESIDUES 13-19 OF CHAIN B WERE NOT SEEN IN THE ELECTRON
REMARK 999 DENSITY.
REMARK 999 THE SIDE CHAINS OF RESIDUES 20, 21, 54, 59, 75, AND 84
REMARK 999 IN CHAIN B WERE NOT SEEN IN THE ELECTRON DENSITY.
DBREF  1EUV A  401   621  GB     1039457  AAB68167       401    621
DBREF  1EUV B   13    98  SWS    Q12306   SMT3_YEAST      13     98
SEQADV 1EUV GLY A  401  GB   1039457   LYS   401 CLONING ARTIFACTS
SEQADV 1EUV SER A  402  GB   1039457   LYS   402 CLONING ARTIFACTS
SEQRES   1 A  221  GLY SER LEU VAL PRO GLU LEU ASN GLU LYS ASP ASP ASP
SEQRES   2 A  221  GLN VAL GLN LYS ALA LEU ALA SER ARG GLU ASN THR GLN
SEQRES   3 A  221  LEU MET ASN ARG ASP ASN ILE GLU ILE THR VAL ARG ASP
SEQRES   4 A  221  PHE LYS THR LEU ALA PRO ARG ARG TRP LEU ASN ASP THR
SEQRES   5 A  221  ILE ILE GLU PHE PHE MET LYS TYR ILE GLU LYS SER THR
SEQRES   6 A  221  PRO ASN THR VAL ALA PHE ASN SER PHE PHE TYR THR ASN
SEQRES   7 A  221  LEU SER GLU ARG GLY TYR GLN GLY VAL ARG ARG TRP MET
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SEQRES   8 A  221  LYS ARG LYS LYS THR GLN ILE ASP LYS LEU ASP LYS ILE
SEQRES   9 A  221  PHE THR PRO ILE ASN LEU ASN GLN SER HIS TRP ALA LEU
SEQRES  10 A  221  GLY ILE ILE ASP LEU LYS LYS LYS THR ILE GLY TYR VAL
SEQRES  11 A  221  ASP SER LEU SER ASN GLY PRO ASN ALA MET SER PHE ALA
SEQRES  12 A  221  ILE LEU THR ASP LEU GLN LYS TYR VAL MET GLU GLU SER
SEQRES  13 A  221  LYS HIS THR ILE GLY GLU ASP PHE ASP LEU ILE HIS LEU
SEQRES  14 A  221  ASP CYS PRO GLN GLN PRO ASN GLY TYR ASP CYS GLY ILE
SEQRES  15 A  221  TYR VAL CYS MET ASN THR LEU TYR GLY SER ALA ASP ALA
SEQRES  16 A  221  PRO LEU ASP PHE ASP TYR LYS ASP ALA ILE ARG MET ARG
SEQRES  17 A  221  ARG PHE ILE ALA HIS LEU ILE LEU THR ASP ALA LEU LYS
SEQRES   1 B   86  GLU VAL LYS PRO GLU VAL LYS PRO GLU THR HIS ILE ASN
SEQRES   2 B   86  LEU LYS VAL SER ASP GLY SER SER GLU ILE PHE PHE LYS
SEQRES   3 B   86  ILE LYS LYS THR THR PRO LEU ARG ARG LEU MET GLU ALA
SEQRES   4 B   86  PHE ALA LYS ARG GLN GLY LYS GLU MET ASP SER LEU ARG
SEQRES   5 B   86  PHE LEU TYR ASP GLY ILE ARG ILE GLN ALA ASP GLN THR
SEQRES   6 B   86  PRO GLU ASP LEU ASP MET GLU ASP ASN ASP ILE ILE GLU
SEQRES   7 B   86  ALA HIS ARG GLU GLN ILE GLY GLY
FORMUL   3  HOH   *432(H2 O1)
HELIX    1   1 ASN A  408  ALA A  420  1                                          13
HELIX    2   2 VAL A  437  LYS A  441  1                                           5
HELIX    3   3 THR A  442  ALA A  444  5                                           3
HELIX    4   4 ASN A  450  THR A  465  1                                          16
HELIX    5   5 SER A  473  GLY A  483  1                                          11
HELIX    6   6 TYR A  484  VAL A  487  5                                           4
HELIX    7   7 MET A  491  LYS A  495  5                                           5
HELIX    8   8 GLN A  497  LEU A  501  5                                           5
HELIX    9   9 ASN A  538  SER A  556  1                                          19
HELIX   10  10 ASP A  579  ALA A  593  1                                          15
HELIX   11  11 ASP A  600  THR A  617  1                                          18
HELIX   12  12 LEU B   45  GLN B   56  1                                          12
HELIX   13  13 GLU B   59  ASP B   61  5                                           3
SHEET    1   A 2 GLN A 426  ARG A 430  0
SHEET    2   A 2 ILE A 433  THR A 436 -1  O  ILE A 433   N  ARG A 430
SHEET    1   B 5 THR A 468  ALA A 470  0
SHEET    2   B 5 LYS A 503  LEU A 510  1  O  LYS A 503   N  VAL A 469
SHEET    3   B 5 HIS A 514  ASP A 521 -1  O  HIS A 514   N  LEU A 510
SHEET    4   B 5 THR A 526  VAL A 530 -1  O  THR A 526   N  ASP A 521
SHEET    5   B 5 ASP A 565  LEU A 569  1  O  ASP A 565   N  ILE A 527
SHEET    1   C 5 GLU B  34  LYS B  40  0
SHEET    2   C 5 HIS B  23  SER B  29 -1  N  ILE B  24   O  ILE B  39
SHEET    3   C 5 ASP B  87  ARG B  93  1  O  ASP B  87   N  LYS B  27
SHEET    4   C 5 LEU B  63  TYR B  67 -1  N  ARG B  64   O  HIS B  92
SHEET    5   C 5 ILE B  70  ARG B  71 -1  O  ILE B  70   N  TYR B  67
LINK         SG  CYS A 580                 C   GLY B  98
CRYST1  125.774   53.167   54.262  90.00  90.00  90.00 P 21 21 2      4
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.007950  0.000000  0.000000        0.00000
SCALE2      0.000000  0.018810  0.000000        0.00000
SCALE3      0.000000  0.000000  0.018430        0.00000
ATOM      1  N   GLY A 401      33.908  16.972  92.970  1.00 40.83           N
ANISOU    1  N   GLY A 401     5308   5152   5054     34   -142    134       N
ATOM      2  CA  GLY A 401      34.959  17.863  92.389  1.00 40.16           C
ANISOU    2  CA  GLY A 401     5199   5101   4959     86   -131     93       C
ATOM      3  C   GLY A 401      34.276  18.853  91.429  1.00 39.45           C
ANISOU    3  C   GLY A 401     5132   5117   4741     96    -84     29       C
ATOM      4  O   GLY A 401      33.765  19.898  91.836  1.00 41.56           O
ANISOU    4  O   GLY A 401     5289   5159   5342    113     -1      8       O
ATOM      5  N   SER A 402      34.308  18.564  90.144  1.00 36.00           N
ANISOU    5  N   SER A 402     4567   4596   4517    206   -292    237       N
ATOM      6  CA  SER A 402      33.593  19.410  89.176  1.00 31.44           C
ANISOU    6  CA  SER A 402     4023   3888   4035    -16   -105     48       C
ATOM      7  C   SER A 402      33.490  18.568  87.917  1.00 28.88           C
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ANISOU    7  C   SER A 402     3621   3603   3750    118   -167    272       C
ATOM      8  O   SER A 402      34.398  17.833  87.545  1.00 30.31           O
ANISOU    8  O   SER A 402     3857   3763   3896    281   -148    218       O
ATOM      9  CB  SER A 402      34.236  20.759  88.859  1.00 30.60           C
ANISOU    9  CB  SER A 402     3984   3744   3898    194   -217    195       C
ATOM     10  OG  SER A 402      33.428  21.458  87.901  1.00 28.46           O
ANISOU   10  OG  SER A 402     3763   3367   3684     85   -148     70       O
ATOM     11  N   LEU A 403      32.358  18.715  87.232  1.00 24.48           N
ANISOU   11  N   LEU A 403     3228   2729   3344     20    -68     91       N
ATOM     12  CA  LEU A 403      32.156  18.045  85.960  1.00 22.66           C
ANISOU   12  CA  LEU A 403     2907   2577   3127     65     11    223       C
ATOM     13  C   LEU A 403      32.648  18.911  84.813  1.00 21.40           C
ANISOU   13  C   LEU A 403     2696   2438   2996     85    -85    152       C
ATOM     14  O   LEU A 403      32.533  18.491  83.671  1.00 21.43           O
ANISOU   14  O   LEU A 403     3033   2035   3075    125     44    179       O
ATOM     15  CB  LEU A 403      30.654  17.761  85.763  1.00 21.94           C
ANISOU   15  CB  LEU A 403     2866   2470   3000     15     85    214       C
ATOM     16  CG  LEU A 403      30.070  16.687  86.706  1.00 22.13           C
ANISOU   16  CG  LEU A 403     2787   2618   3003     68    171    266       C
ATOM     17  CD1 LEU A 403      28.607  16.437  86.413  1.00 23.95           C
ANISOU   17  CD1 LEU A 403     3074   2778   3249    -32    -70     20       C
ATOM     18  CD2 LEU A 403      30.897  15.404  86.513  1.00 23.40           C
ANISOU   18  CD2 LEU A 403     3198   2409   3283    -36     69     60       C
ATOM     19  N   VAL A 404      33.143  20.116  85.092  1.00 22.43           N
ANISOU   19  N   VAL A 404     2884   2486   3153    114   -106    152       N
ATOM     20  CA  VAL A 404      33.683  20.963  84.021  1.00 22.06           C
ANISOU   20  CA  VAL A 404     2880   2453   3050     80    -22     91       C
ATOM     21  C   VAL A 404      35.197  20.906  84.138  1.00 22.63           C
ANISOU   21  C   VAL A 404     3081   2515   3001    138   -108    249       C
ATOM     22  O   VAL A 404      35.785  21.433  85.067  1.00 24.07           O
ANISOU   22  O   VAL A 404     2846   3020   3279    128   -221    178       O
ATOM     23  CB  VAL A 404      33.147  22.416  84.244  1.00 21.98           C
ANISOU   23  CB  VAL A 404     2895   2505   2951    158    -13    131       C
ATOM     24  CG1 VAL A 404      33.678  23.330  83.137  1.00 21.57           C
ANISOU   24  CG1 VAL A 404     2633   2638   2926     59    -25    132       C
ATOM     25  CG2 VAL A 404      31.636  22.469  84.333  1.00 20.47           C
ANISOU   25  CG2 VAL A 404     2813   2171   2794    -47    -76     44       C
ATOM     26  N   PRO A 405      35.860  20.317  83.172  1.00 23.66           N
ANISOU   26  N   PRO A 405     3008   2745   3235     89     31    168       N
ATOM     27  CA  PRO A 405      37.313  20.171  83.266  1.00 26.77           C
ANISOU   27  CA  PRO A 405     3176   3461   3535    116    -32     99       C
ATOM     28  C   PRO A 405      38.073  21.419  82.867  1.00 30.16           C
ANISOU   28  C   PRO A 405     3742   3725   3992    -99     -6    186       C
ATOM     29  O   PRO A 405      37.569  22.254  82.115  1.00 31.05           O
ANISOU   29  O   PRO A 405     3572   4012   4213    133    -42    218       O
ATOM     30  CB  PRO A 405      37.602  19.013  82.310  1.00 27.12           C
ANISOU   30  CB  PRO A 405     3320   3480   3506     35    -40     78       C
ATOM     31  CG  PRO A 405      36.575  19.165  81.253  1.00 26.08           C
ANISOU   31  CG  PRO A 405     3445   3222   3241     76     27    100       C
ATOM     32  CD  PRO A 405      35.322  19.665  81.962  1.00 24.17           C
ANISOU   32  CD  PRO A 405     3120   2926   3135     87    -29    248       C
ATOM     33  N   GLU A 406      39.331  21.452  83.308  1.00 32.15           N
ANISOU   33  N   GLU A 406     3743   4267   4205     62    -82     84       N
ATOM     34  CA  GLU A 406      40.213  22.546  82.896  1.00 34.41           C
ANISOU   34  CA  GLU A 406     4328   4297   4449    -26     60    111       C
ATOM     35  C   GLU A 406      40.962  22.009  81.678  1.00 33.20           C
ANISOU   35  C   GLU A 406     4044   4240   4329    -11    -78    122       C
ATOM     36  O   GLU A 406      41.302  20.813  81.564  1.00 34.60           O
ANISOU   36  O   GLU A 406     4388   4326   4431     23     75     21       O
ATOM     37  CB  GLU A 406      41.151  22.996  84.009  1.00 38.62           C
ANISOU   37  CB  GLU A 406     4774   5087   4814     72   -213    -63       C
ATOM     38  CG  GLU A 406      42.199  24.009  83.657  1.00 42.90           C
ANISOU   38  CG  GLU A 406     5265   5561   5476   -144     28     90       C
ATOM     39  CD  GLU A 406      42.099  25.492  83.825  1.00 46.53           C
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ANISOU   39  CD  GLU A 406     5937   5757   5985     39     55    -58       C
ATOM     40  OE1 GLU A 406      41.014  26.121  83.840  1.00 47.63           O
ANISOU   40  OE1 GLU A 406     5807   6185   6105     64    -66     -3       O
ATOM     41  OE2 GLU A 406      43.201  26.138  83.932  1.00 48.05           O
ANISOU   41  OE2 GLU A 406     5984   6029   6244    -25    -38   -141       O
ATOM     42  N   LEU A 407      41.204  22.874  80.717  1.00 30.75           N
ANISOU   42  N   LEU A 407     3597   4095   3993     67   -165    -26       N
ATOM     43  CA  LEU A 407      41.903  22.531  79.517  1.00 30.07           C
ANISOU   43  CA  LEU A 407     3494   3990   3943    115   -134     65       C
ATOM     44  C   LEU A 407      43.435  22.550  79.725  1.00 31.27           C
ANISOU   44  C   LEU A 407     3497   4217   4169      2   -112     20       C
ATOM     45  O   LEU A 407      43.881  23.391  80.490  1.00 30.61           O
ANISOU   45  O   LEU A 407     3258   4132   4240     66   -101    -21       O
ATOM     46  CB  LEU A 407      41.649  23.568  78.415  1.00 28.26           C
ANISOU   46  CB  LEU A 407     3228   3746   3763     29   -113    -33       C
ATOM     47  CG  LEU A 407      40.187  23.605  77.902  1.00 26.89           C
ANISOU   47  CG  LEU A 407     3178   3570   3469    149    -77      3       C
ATOM     48  CD1 LEU A 407      40.175  24.443  76.618  1.00 26.19           C
ANISOU   48  CD1 LEU A 407     3100   3351   3499     61     37     19       C
ATOM     49  CD2 LEU A 407      39.686  22.202  77.667  1.00 26.73           C
ANISOU   49  CD2 LEU A 407     2994   3575   3589     89    -56    128       C
ATOM     50  N   ASN A 408      44.132  21.677  79.008  1.00 33.58           N
ANISOU   50  N   ASN A 408     4138   4293   4328    106    -18    -20       N
ATOM     51  CA  ASN A 408      45.598  21.797  79.140  1.00 35.58           C
ANISOU   51  CA  ASN A 408     4173   4655   4692     55    -49    -36       C
ATOM     52  C   ASN A 408      46.002  23.026  78.339  1.00 36.95           C
ANISOU   52  C   ASN A 408     4461   4781   4796     35      1     52       C
ATOM     53  O   ASN A 408      45.213  23.564  77.556  1.00 36.50           O
ANISOU   53  O   ASN A 408     4277   4887   4704    -25     25      6       O
ATOM     54  CB  ASN A 408      46.331  20.558  78.694  1.00 36.63           C
ANISOU   54  CB  ASN A 408     4492   4717   4708    200     -6    -31       C
ATOM     55  CG  ASN A 408      46.048  20.146  77.271  1.00 36.32           C
ANISOU   55  CG  ASN A 408     4346   4754   4701     89     15    -13       C
ATOM     56  OD1 ASN A 408      45.999  21.002  76.388  1.00 36.87           O
ANISOU   56  OD1 ASN A 408     4442   4779   4790    159    114     -1       O
ATOM     57  ND2 ASN A 408      45.870  18.847  77.051  1.00 37.25           N
ANISOU   57  ND2 ASN A 408     4626   4785   4744    155     54    -41       N
ATOM     58  N   GLU A 409      47.255  23.461  78.456  1.00 38.07           N
ANISOU   58  N   GLU A 409     4528   4910   5025     46    -64    -21       N
ATOM     59  CA  GLU A 409      47.684  24.665  77.761  1.00 39.20           C
ANISOU   59  CA  GLU A 409     4768   5065   5059     -6     49     40       C
ATOM     60  C   GLU A 409      47.541  24.565  76.260  1.00 37.19           C
ANISOU   60  C   GLU A 409     4244   4835   5052   -106    -66    -31       C
ATOM     61  O   GLU A 409      47.235  25.552  75.594  1.00 36.14           O
ANISOU   61  O   GLU A 409     3935   4839   4957    -85    -99   -104       O
ATOM     62  CB  GLU A 409      49.144  24.975  78.132  1.00 42.63           C
ANISOU   62  CB  GLU A 409     4977   5672   5550     27   -114    -47       C
ATOM     63  CG  GLU A 409      49.702  26.229  77.505  1.00 46.82           C
ANISOU   63  CG  GLU A 409     5820   5939   6031    -76     34    161       C
ATOM     64  CD  GLU A 409      49.707  27.455  78.393  1.00 49.99           C
ANISOU   64  CD  GLU A 409     6365   6256   6375      1     19    -79       C
ATOM     65  OE1 GLU A 409      49.064  27.396  79.471  1.00 52.03           O
ANISOU   65  OE1 GLU A 409     6556   6681   6531     -7    129     30       O
ATOM     66  OE2 GLU A 409      50.356  28.472  78.036  1.00 51.15           O
ANISOU   66  OE2 GLU A 409     6452   6422   6560    -59     78     69       O
ATOM     67  N   LYS A 410      47.851  23.413  75.679  1.00 36.76           N
ANISOU   67  N   LYS A 410     4172   4828   4967     47    -73     41       N
ATOM     68  CA  LYS A 410      47.782  23.220  74.238  1.00 38.50           C
ANISOU   68  CA  LYS A 410     4491   5115   5022     47    -84      8       C
ATOM     69  C   LYS A 410      46.335  23.398  73.741  1.00 36.66           C
ANISOU   69  C   LYS A 410     4361   4727   4840     81     48     46       C
ATOM     70  O   LYS A 410      46.059  24.076  72.753  1.00 35.34           O
ANISOU   70  O   LYS A 410     3997   4611   4820    113      2    -50       O
ATOM     71  CB  LYS A 410      48.361  21.841  73.927  1.00 41.63           C
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ANISOU   71  CB  LYS A 410     5150   5213   5454    181     25     18       C
ATOM     72  CG  LYS A 410      47.458  20.740  73.457  1.00 44.64           C
ANISOU   72  CG  LYS A 410     5565   5594   5803    -20    -68    -91       C
ATOM     73  CD  LYS A 410      47.498  19.428  74.240  1.00 46.31           C
ANISOU   73  CD  LYS A 410     5878   5778   5938      6     16     48       C
ATOM     74  CE  LYS A 410      46.695  18.362  73.510  1.00 47.17           C
ANISOU   74  CE  LYS A 410     6037   5854   6030    -11      2    -47       C
ATOM     75  NZ  LYS A 410      45.610  17.732  74.308  1.00 47.79           N
ANISOU   75  NZ  LYS A 410     6050   6032   6076     36     63    -48       N
ATOM     76  N   ASP A 411      45.423  22.744  74.439  1.00 35.18           N
ANISOU   76  N   ASP A 411     4135   4526   4707    148    -61     18       N
ATOM     77  CA  ASP A 411      43.998  22.806  74.077  1.00 32.85           C
ANISOU   77  CA  ASP A 411     3975   4136   4370    174     39      7       C
ATOM     78  C   ASP A 411      43.466  24.227  74.250  1.00 32.37           C
ANISOU   78  C   ASP A 411     3909   4131   4259    142      3     46       C
ATOM     79  O   ASP A 411      42.678  24.657  73.393  1.00 29.80           O
ANISOU   79  O   ASP A 411     3381   3767   4173    396    227   -138       O
ATOM     80  CB  ASP A 411      43.197  21.774  74.857  1.00 32.86           C
ANISOU   80  CB  ASP A 411     4022   4211   4254    108    -15     22       C
ATOM     81  CG  ASP A 411      43.488  20.337  74.494  1.00 33.23           C
ANISOU   81  CG  ASP A 411     4008   4275   4344    135    -59     11       C
ATOM     82  OD1 ASP A 411      44.035  20.081  73.411  1.00 35.03           O
ANISOU   82  OD1 ASP A 411     4439   4490   4382    246    -69     26       O
ATOM     83  OD2 ASP A 411      43.189  19.384  75.244  1.00 33.96           O
ANISOU   83  OD2 ASP A 411     4179   4148   4576    132   -130     -3       O
ATOM     84  N   ASP A 412      43.863  24.920  75.299  1.00 32.19           N
ANISOU   84  N   ASP A 412     3713   4205   4314     87     46     33       N
ATOM     85  CA  ASP A 412      43.434  26.311  75.507  1.00 33.69           C
ANISOU   85  CA  ASP A 412     3959   4210   4631     40     98     88       C
ATOM     86  C   ASP A 412      43.948  27.194  74.377  1.00 33.14           C
ANISOU   86  C   ASP A 412     3915   4285   4392     36     52      9       C
ATOM     87  O   ASP A 412      43.258  28.083  73.893  1.00 32.19           O
ANISOU   87  O   ASP A 412     3706   4220   4306   -124     86     76       O
ATOM     88  CB  ASP A 412      43.889  26.811  76.859  1.00 37.61           C
ANISOU   88  CB  ASP A 412     4614   4918   4758    -20    -31     11       C
ATOM     89  CG  ASP A 412      43.634  28.229  77.299  1.00 42.22           C
ANISOU   89  CG  ASP A 412     5493   5127   5420     76    -11    -79       C
ATOM     90  OD1 ASP A 412      43.240  29.189  76.599  1.00 41.69           O
ANISOU   90  OD1 ASP A 412     5302   5222   5316     61    -25    -61       O
ATOM     91  OD2 ASP A 412      43.693  28.409  78.555  1.00 45.86           O
ANISOU   91  OD2 ASP A 412     6083   5826   5515     31     37   -123       O
ATOM     92  N   ASP A 413      45.186  26.985  73.919  1.00 33.23           N
ANISOU   92  N   ASP A 413     3947   4297   4380     21    128    -36       N
ATOM     93  CA  ASP A 413      45.726  27.835  72.859  1.00 33.18           C
ANISOU   93  CA  ASP A 413     3965   4321   4322     33    143    -40       C
ATOM     94  C   ASP A 413      44.980  27.675  71.552  1.00 31.01           C
ANISOU   94  C   ASP A 413     3436   4091   4253    101    290      1       C
ATOM     95  O   ASP A 413      44.794  28.636  70.810  1.00 29.88           O
ANISOU   95  O   ASP A 413     3073   4219   4060     21    307     40       O
ATOM     96  CB  ASP A 413      47.209  27.472  72.638  1.00 36.39           C
ANISOU   96  CB  ASP A 413     4115   4850   4860    115    172    -14       C
ATOM     97  CG  ASP A 413      48.100  28.137  73.665  1.00 39.77           C
ANISOU   97  CG  ASP A 413     4814   5190   5107    -49    -46    -75       C
ATOM     98  OD1 ASP A 413      47.634  29.045  74.401  1.00 41.39           O
ANISOU   98  OD1 ASP A 413     4961   5376   5390     84     25   -129       O
ATOM     99  OD2 ASP A 413      49.289  27.737  73.710  1.00 40.98           O
ANISOU   99  OD2 ASP A 413     4919   5314   5337     34     -4    -36       O
ATOM    100  N   GLN A 414      45.505  26.453  71.311  1.00 30.31           N
ANISOU  100  N   GLN A 414     3359   4105   4050     75    261   -112       N
ATOM    101  CA  GLN A 414      43.725  26.129  70.124  1.00 30.58           C
ANISOU  101  CA  GLN A 414     3461   4162   3996    104    183     27       C
ATOM    102  C   GLN A 414      42.429  26.940  70.167  1.00 28.35           C
ANISOU  102  C   GLN A 414     3389   3698   3685    -51     97    -26       C
ATOM    103  O   GLN A 414      42.049  27.542  69.168  1.00 27.07           O
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Deposited on 08/24/2001

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ANISOU  103  O   GLN A 414     2863   3826   3597     16    297    -56       O
ATOM    104  CB  GLN A 414      43.437  24.628  70.097  1.00 33.29           C
ANISOU  104  CB  GLN A 414     3960   4231   4459     68    140    -46       C
ATOM    105  CG  GLN A 414      42.767  24.142  68.831  1.00 36.44           C
ANISOU  105  CG  GLN A 414     4523   4811   4510     57      2    -86       C
ATOM    106  CD  GLN A 414      42.332  22.694  68.807  1.00 38.97           C
ANISOU  106  CD  GLN A 414     4948   4869   4990     37     17    -30       C
ATOM    107  OE1 GLN A 414      42.176  21.994  69.813  1.00 39.33           O
ANISOU  107  OE1 GLN A 414     4907   5059   4978    145    130    -10       O
ATOM    108  NE2 GLN A 414      42.089  22.204  67.581  1.00 40.14           N
ANISOU  108  NE2 GLN A 414     5108   5146   4995     97     38    -99       N
ATOM    109  N   VAL A 415      41.776  26.933  71.336  1.00 27.93           N
ANISOU  109  N   VAL A 415     3254   3688   3669     24    120   -105       N
ATOM    110  CA  VAL A 415      40.577  27.777  71.508  1.00 27.64           C
ANISOU  110  CA  VAL A 415     3407   3565   3531     33    157     56       C
ATOM    111  C   VAL A 415      40.894  29.248  71.236  1.00 28.30           C
ANISOU  111  C   VAL A 415     3498   3560   3696     50     97    -32       C
ATOM    112  O   VAL A 415      40.207  29.882  70.438  1.00 26.80           O
ANISOU  112  O   VAL A 415     3141   3682   3361   -139    318     40       O
ATOM    113  CB  VAL A 415      40.021  27.623  72.938  1.00 26.21           C
ANISOU  113  CB  VAL A 415     3199   3290   3470     81    169    -84       C
ATOM    114  CG1 VAL A 415      38.926  28.661  73.191  1.00 24.26           C
ANISOU  114  CG1 VAL A 415     3073   3127   3018     55    100    -31       C
ATOM    115  CG2 VAL A 415      39.500  26.210  73.170  1.00 26.40           C
ANISOU  115  CG2 VAL A 415     3219   3299   3513     87    187   -135       C
ATOM    116  N   GLN A 416      41.937  29.807  71.834  1.00 30.21           N
ANISOU  116  N   GLN A 416     3553   3958   3968    -40     20    -38       N
ATOM    117  CA  GLN A 416      42.305  31.223  71.647  1.00 32.66           C
ANISOU  117  CA  GLN A 416     3944   4116   4350    -84     87      5       C
ATOM    118  C   GLN A 416      42.582  31.547  70.189  1.00 32.92           C
ANISOU  118  C   GLN A 416     3868   4255   4385   -173     37     64       C
ATOM    119  O   GLN A 416      42.093  32.561  69.677  1.00 32.32           O
ANISOU  119  O   GLN A 416     3600   4158   4521   -304    242    144       O
ATOM    120  CB  GLN A 416      43.441  31.586  72.610  1.00 34.16           C
ANISOU  120  CB  GLN A 416     4088   4399   4493    -71      6    -42       C
ATOM    121  CG  GLN A 416      43.730  33.065  72.837  1.00 35.92           C
ANISOU  121  CG  GLN A 416     4471   4456   4721    -68     78    -51       C
ATOM    122  CD  GLN A 416      42.815  33.729  73.852  1.00 36.77           C
ANISOU  122  CD  GLN A 416     4614   4558   4798    -51    112   -100       C
ATOM    123  OE1 GLN A 416      41.740  33.219  74.178  1.00 35.20           O
ANISOU  123  OE1 GLN A 416     4475   4258   4641     -6     99    -75       O
ATOM    124  NE2 GLN A 416      43.257  34.888  74.359  1.00 36.70           N
ANISOU  124  NE2 GLN A 416     4667   4464   4813    -11      3      1       N
ATOM    125  N   LYS A 417      43.251  30.665  69.434  1.00 34.04           N
ANISOU  125  N   LYS A 417     4038   4303   4592   -131     97    -37       N
ATOM    126  CA  LYS A 417      43.497  30.890  68.012  1.00 35.76           C
ANISOU  126  CA  LYS A 417     4375   4586   4628   -163     11     63       C
ATOM    127  C   LYS A 417      42.222  30.925  67.179  1.00 34.58           C
ANISOU  127  C   LYS A 417     4260   4343   4536    -93    100    111       C
ATOM    128  O   LYS A 417      42.025  31.750  66.289  1.00 34.18           O
ANISOU  128  O   LYS A 417     4068   4441   4476   -196    163    181       O
ATOM    129  CB  LYS A 417      44.337  29.768  67.395  1.00 38.84           C
ANISOU  129  CB  LYS A 417     4878   4805   5074    -25    150    -58       C
ATOM    130  CG  LYS A 417      45.608  29.400  68.112  1.00 42.20           C
ANISOU  130  CG  LYS A 417     5220   5398   5416     10   -105     56       C
ATOM    131  CD  LYS A 417      46.384  28.344  67.308  1.00 44.53           C
ANISOU  131  CD  LYS A 417     5611   5583   5725     80     66    -21       C
ATOM    132  CE  LYS A 417      47.848  28.366  67.760  1.00 46.02           C
ANISOU  132  CE  LYS A 417     5687   5874   5924     25    -24     35       C
ATOM    133  NZ  LYS A 417      48.448  29.714  67.513  1.00 46.73           N
ANISOU  133  NZ  LYS A 417     5835   5884   6035      5      2     -4       N
ATOM    134  N   ALA A 418      41.342  29.957  67.464  1.00 33.25           N
ANISOU  134  N   ALA A 418     4054   4272   4309    -34     52     71       N
ATOM    135  CA  ALA A 418      40.061  29.907  66.748  1.00 31.26           C
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ANISOU  135  CA  ALA A 418     3863   4041   3973   -119    175     18       C
ATOM    136  C   ALA A 418      39.239  31.154  67.014  1.00 30.31           C
ANISOU  136  C   ALA A 418     3761   3858   3898   -223     55    116       C
ATOM    137  O   ALA A 418      38.595  31.695  66.130  1.00 28.84           O
ANISOU  137  O   ALA A 418     3437   3784   3737   -282    277     98       O
ATOM    138  CB  ALA A 418      39.321  28.633  67.148  1.00 30.90           C
ANISOU  138  CB  ALA A 418     3821   3956   3965    -83     79     14       C
ATOM    139  N   LEU A 419      39.237  31.719  68.222  1.00 30.33           N
ANISOU  139  N   LEU A 419     3656   3838   4029   -309    186     10       N
ATOM    140  CA  LEU A 419      38.502  32.928  68.551  1.00 32.41           C
ANISOU  140  CA  LEU A 419     3996   4102   4216    -64     20    -35       C
ATOM    141  C   LEU A 419      39.056  34.157  67.827  1.00 35.75           C
ANISOU  141  C   LEU A 419     4660   4318   4604   -119     15    148       C
ATOM    142  O   LEU A 419      38.334  35.129  67.632  1.00 36.41           O
ANISOU  142  O   LEU A 419     4665   4311   4857    -76    125     39       O
ATOM    143  CB  LEU A 419      38.553  33.202  70.049  1.00 31.38           C
ANISOU  143  CB  LEU A 419     3959   3825   4141    -96      9      8       C
ATOM    144  CG  LEU A 419      37.792  32.275  70.985  1.00 29.76           C
ANISOU  144  CG  LEU A 419     3581   3926   3801    -17    -12    -50       C
ATOM    145  CD1 LEU A 419      38.175  32.531  72.435  1.00 29.11           C
ANISOU  145  CD1 LEU A 419     3735   3547   3780     -9    -39    -54       C
ATOM    146  CD2 LEU A 419      36.278  32.458  70.802  1.00 28.85           C
ANISOU  146  CD2 LEU A 419     3560   3738   3664     16    -41   -129       C
ATOM    147  N   ALA A 420      40.310  34.071  67.420  1.00 38.82           N
ANISOU  147  N   ALA A 420     4696   4998   5057     20     22    -23       N
ATOM    148  CA  ALA A 420      40.925  35.169  66.695  1.00 42.84           C
ANISOU  148  CA  ALA A 420     5345   5283   5649    -74     94    198       C
ATOM    149  C   ALA A 420      40.876  34.939  65.197  1.00 46.54           C
ANISOU  149  C   ALA A 420     5897   5976   5809     72     59     70       C
ATOM    150  O   ALA A 420      41.473  35.806  64.528  1.00 46.77           O
ANISOU  150  O   ALA A 420     5836   5990   5944    -58     37     24       O
ATOM    151  CB  ALA A 420      42.383  35.300  67.133  1.00 42.55           C
ANISOU  151  CB  ALA A 420     5357   5328   5484    -26     68    112       C
ATOM    152  N   SER A 421      39.687  34.907  62.460  1.00 57.01           C
ANISOU  152  N   SER A 421     7152   7227   7282    115    -91      7       C
ATOM    153  CA  SER A 421      40.428  33.802  63.210  1.00 54.60           C
ANISOU  153  CA  SER A 421     6935   7048   6764    -44     46    -15       C
ATOM    154  C   SER A 421      39.687  34.907  62.460  1.00 57.01           C
ANISOU  154  C   SER A 421     7152   7227   7282    115    -91      7       C
ATOM    155  O   SER A 421      38.600  35.374  62.710  1.00 56.19           O
ANISOU  155  O   SER A 421     7102   7171   7076    -31    -51     -7       O
ATOM    156  CB  SER A 421      40.370  32.496  62.468  1.00 56.08           C
ANISOU  156  CB  SER A 421     7128   7019   7159    -29     39    -43       C
ATOM    157  OG  SER A 421      39.715  32.602  61.206  1.00 57.68           O
ANISOU  157  OG  SER A 421     7242   7382   7291    -26    -32     29       O
ATOM    158  N   ARG A 422      40.514  35.340  61.508  1.00 60.66           N
ANISOU  158  N   ARG A 422     7599   7808   7640    -44     96    -22       N
ATOM    159  CA  ARG A 422      40.244  36.346  60.509  1.00 63.35           C
ANISOU  159  CA  ARG A 422     8092   7994   7986     82     32    148       C
ATOM    160  C   ARG A 422      39.395  35.667  59.422  1.00 65.36           C
ANISOU  160  C   ARG A 422     8264   8317   8251     -5    -44     27       C
ATOM    161  O   ARG A 422      39.766  35.074  58.416  1.00 66.33           O
ANISOU  161  O   ARG A 422     8454   8401   8346     39     22    -11       O
ATOM    162  CB  ARG A 422      40.997  37.273  60.466  0.00 59.92           C
ATOM    163  CG  ARG A 422      40.723  38.706  60.039  0.00 56.99           C
ATOM    164  CD  ARG A 422      40.341  39.575  61.227  0.00 54.62           C
ATOM    165  NE  ARG A 422      40.086  40.956  60.834  0.00 53.35           N
ATOM    166  CZ  ARG A 422      39.736  41.924  61.676  0.00 51.98           C
ATOM    167  NH1 ARG A 422      39.600  41.659  62.970  0.00 52.27           N
ATOM    168  NH2 ARG A 422      39.524  43.153  61.226  0.00 52.14           N
ATOM    169  N   GLU A 423      38.106  35.761  59.692  1.00 65.38           N
ANISOU  169  N   GLU A 423     8268   8334   8238     -4      9     42       N
ATOM    170  CA  GLU A 423      36.966  35.458  58.893  1.00 65.22           C
ANISOU  170  CA  GLU A 423     8230   8200   8349    -55     16     23       C
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ATOM    171  C   GLU A 423      36.092  34.307  59.292  1.00 63.05           C
ANISOU  171  C   GLU A 423     7921   8063   7972     66    -33     -5       C
ATOM    172  O   GLU A 423      36.424  33.404  60.046  1.00 62.56           O
ANISOU  172  O   GLU A 423     7907   7979   7885    -22      1    -22       O
ATOM    173  CB  GLU A 423      37.262  35.696  57.389  1.00 67.48           C
ANISOU  173  CB  GLU A 423     8545   8674   8420    -14     34     21       C
ATOM    174  CG  GLU A 423      37.198  37.195  57.260  1.00 69.65           C
ANISOU  174  CG  GLU A 423     8868   8736   8862     -4     -1    -25       C
ATOM    175  CD  GLU A 423      37.431  38.247  56.269  1.00 70.95           C
ANISOU  175  CD  GLU A 423     9060   8927   8969    -18     36     61       C
ATOM    176  OE1 GLU A 423      36.914  38.204  55.128  1.00 71.70           O
ANISOU  176  OE1 GLU A 423     9103   9102   9039    -12    -18      6       O
ATOM    177  OE2 GLU A 423      38.135  39.235  56.635  1.00 71.54           O
ANISOU  177  OE2 GLU A 423     9115   9008   9058    -42      5    -11       O
ATOM    178  N   ASN A 424      34.827  34.492  58.891  1.00 60.44           N
ANISOU  178  N   ASN A 424     7734   7603   7627    -93    107     30       N
ATOM    179  CA  ASN A 424      33.724  33.638  59.273  1.00 57.76           C
ANISOU  179  CA  ASN A 424     7432   7276   7238     44      2    -65       C
ATOM    180  C   ASN A 424      33.628  32.341  58.492  1.00 55.12           C
ANISOU  180  C   ASN A 424     6949   7060   6936     41     52    111       C
ATOM    181  O   ASN A 424      32.775  32.089  57.660  1.00 55.76           O
ANISOU  181  O   ASN A 424     7065   7155   6965    -61     44      6       O
ATOM    182  CB  ASN A 424      32.402  34.424  59.250  1.00 57.84           C
ANISOU  182  CB  ASN A 424     7352   7310   7313    -13     37     17       C
ATOM    183  CG  ASN A 424      31.332  33.693  60.060  1.00 57.45           C
ANISOU  183  CG  ASN A 424     7353   7259   7216      5     34     -2       C
ATOM    184  OD1 ASN A 424      30.127  33.860  59.837  1.00 57.50           O
ANISOU  184  OD1 ASN A 424     7350   7270   7227     25     72      0       O
ATOM    185  ND2 ASN A 424      31.807  32.870  60.983  1.00 56.42           N
ANISOU  185  ND2 ASN A 424     7196   7128   7113    -30     63    -45       N
ATOM    186  N   THR A 425      34.530  31.452  58.852  1.00 51.97           N
ANISOU  186  N   THR A 425     6741   6514   6491   -139    151    -38       N
ATOM    187  CA  THR A 425      34.702  30.138  58.285  1.00 49.63           C
ANISOU  187  CA  THR A 425     6342   6305   6208   -147    138    134       C
ATOM    188  C   THR A 425      33.915  29.109  59.092  1.00 45.80           C
ANISOU  188  C   THR A 425     5959   5706   5738    -10     -1   -132       C
ATOM    189  O   THR A 425      33.537  29.348  60.235  1.00 43.73           O
ANISOU  189  O   THR A 425     5602   5307   5705    -99    100      1       O
ATOM    190  CB  THR A 425      36.205  29.790  58.329  1.00 51.23           C
ANISOU  190  CB  THR A 425     6461   6520   6486      2     46     16       C
ATOM    191  OG1 THR A 425      36.604  29.503  59.677  1.00 52.07           O
ANISOU  191  OG1 THR A 425     6610   6666   6509     10     42     32       O
ATOM    192  CG2 THR A 425      37.045  30.974  57.854  1.00 51.68           C
ANISOU  192  CG2 THR A 425     6550   6545   6540    -14     56     50       C
ATOM    193  N   GLN A 426      33.658  27.974  58.466  1.00 42.17           N
ANISOU  193  N   GLN A 426     5411   5391   5223    -37    118    127       N
ATOM    194  CA  GLN A 426      32.982  26.855  59.105  1.00 39.41           C
ANISOU  194  CA  GLN A 426     5005   5086   4884     37     -3    -56       C
ATOM    195  C   GLN A 426      33.993  26.128  59.982  1.00 37.10           C
ANISOU  195  C   GLN A 426     4776   4805   4515    -74    159    -55       C
ATOM    196  O   GLN A 426      35.066  25.714  59.503  1.00 37.82           O
ANISOU  196  O   GLN A 426     4897   4908   4565     -1    262   -142       O
ATOM    197  CB  GLN A 426      32.450  25.920  58.005  1.00 39.00           C
ANISOU  197  CB  GLN A 426     4990   5007   4823     -6     80    -25       C
ATOM    198  CG  GLN A 426      31.402  24.930  58.474  1.00 39.95           C
ANISOU  198  CG  GLN A 426     5175   4998   5006    -84     66    -24       C
ATOM    199  CD  GLN A 426      31.088  23.834  57.460  1.00 39.53           C
ANISOU  199  CD  GLN A 426     5106   5002   4912     -5    105    -14       C
ATOM    200  OE1 GLN A 426      31.921  22.931  57.334  1.00 39.47           O
ANISOU  200  OE1 GLN A 426     5229   4871   4896    -25     72    -23       O
ATOM    201  NE2 GLN A 426      29.942  23.904  56.798  1.00 39.22           N
ANISOU  201  NE2 GLN A 426     5148   4927   4828    -79    111    -10       N
ATOM    202  N   LEU A 427      33.732  25.962  61.274  1.00 33.29           N
ANISOU  202  N   LEU A 427     4191   4150   4307      0     87   -103       N
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ATOM    203  CA  LEU A 427      34.639  25.301  62.188  1.00 31.60           C
ANISOU  203  CA  LEU A 427     4120   3952   3935    -70    202   -138       C
ATOM    204  C   LEU A 427      34.269  23.842  62.475  1.00 30.46           C
ANISOU  204  C   LEU A 427     3987   3948   3639     13    129    -45       C
ATOM    205  O   LEU A 427      35.135  23.106  62.938  1.00 30.00           O
ANISOU  205  O   LEU A 427     3925   3879   3595    168    301   -167       O
ATOM    206  CB  LEU A 427      34.701  26.001  63.560  1.00 30.35           C
ANISOU  206  CB  LEU A 427     3809   3923   3800     -1    112    -28       C
ATOM    207  CG  LEU A 427      35.428  27.332  63.595  1.00 30.36           C
ANISOU  207  CG  LEU A 427     3871   3888   3779     20     61    -68       C
ATOM    208  CD1 LEU A 427      35.288  27.954  64.974  1.00 29.52           C
ANISOU  208  CD1 LEU A 427     3708   3678   3830      1     87   -102       C
ATOM    209  CD2 LEU A 427      36.894  27.140  63.235  1.00 30.35           C
ANISOU  209  CD2 LEU A 427     3901   3837   3792    -12    124    -47       C
ATOM    210  N   MET A 428      32.988  23.532  62.301  1.00 29.77           N
ANISOU  210  N   MET A 428     3951   3747   3615     20    240    -87       N
ATOM    211  CA  MET A 428      32.508  22.182  62.580  1.00 29.75           C
ANISOU  211  CA  MET A 428     3885   3803   3617     -2    150    -45       C
ATOM    212  C   MET A 428      31.203  21.991  61.818  1.00 30.03           C
ANISOU  212  C   MET A 428     3819   3836   3756    -31    133    -27       C
ATOM    213  O   MET A 428      30.451  22.931  61.548  1.00 28.48           O
ANISOU  213  O   MET A 428     3602   3655   3564   -152    286   -228       O
ATOM    214  CB  MET A 428      32.292  22.019  64.088  1.00 29.26           C
ANISOU  214  CB  MET A 428     3881   3633   3605     26    154    -38       C
ATOM    215  CG  MET A 428      32.239  20.562  64.570  1.00 28.39           C
ANISOU  215  CG  MET A 428     3766   3616   3407     31    240    -80       C
ATOM    216  SD  MET A 428      31.278  20.440  66.111  1.00 25.70           S
ANISOU  216  SD  MET A 428     3358   3041   3368     36    234   -505       S
ATOM    217  CE  MET A 428      29.628  20.532  65.423  1.00 26.43           C
ANISOU  217  CE  MET A 428     3500   3193   3348     39     38   -197       C
ATOM    218  N   ASN A 429      30.969  20.760  61.384  1.00 30.83           N
ANISOU  218  N   ASN A 429     3955   3869   3892     41    153   -130       N
ATOM    219  CA  ASN A 429      29.748  20.434  60.663  1.00 31.92           C
ANISOU  219  CA  ASN A 429     3919   4050   4161     85     98    -89       C
ATOM    220  C   ASN A 429      29.519  18.945  60.884  1.00 31.94           C
ANISOU  220  C   ASN A 429     3957   4076   4104     32    119    -53       C
ATOM    221  O   ASN A 429      30.201  18.120  60.258  1.00 33.09           O
ANISOU  221  O   ASN A 429     4188   4226   4160     42    182   -215       O
ATOM    222  CB  ASN A 429      29.797  20.803  59.196  1.00 34.07           C
ANISOU  222  CB  ASN A 429     4403   4315   4229     74    142    -37       C
ATOM    223  CG  ASN A 429      28.451  20.675  58.523  1.00 36.74           C
ANISOU  223  CG  ASN A 429     4631   4747   4583     26    -52    -56       C
ATOM    224  OD1 ASN A 429      27.419  20.747  59.208  1.00 37.57           O
ANISOU  224  OD1 ASN A 429     4722   4952   4602     43    -13   -104       O
ATOM    225  ND2 ASN A 429      28.429  20.485  57.210  1.00 37.30           N
ANISOU  225  ND2 ASN A 429     4892   4698   4583     83     44    -16       N
ATOM    226  N   ARG A 430      28.680  18.646  61.861  1.00 30.73           N
ANISOU  226  N   ARG A 430     3821   3885   3969     71    102   -123       N
ATOM    227  CA  ARG A 430      28.476  17.228  62.191  1.00 32.06           C
ANISOU  227  CA  ARG A 430     4078   3965   4140    -24    191   -105       C
ATOM    228  C   ARG A 430      27.136  17.026  62.862  1.00 32.39           C
ANISOU  228  C   ARG A 430     3955   4076   4278      5     76   -137       C
ATOM    229  O   ARG A 430      26.751  17.893  63.646  1.00 31.05           O
ANISOU  229  O   ARG A 430     3572   3968   4258      4     35   -149       O
ATOM    230  CB  ARG A 430      29.612  16.842  63.128  1.00 33.68           C
ANISOU  230  CB  ARG A 430     4203   4287   4308    -62     46    -42       C
ATOM    231  CG  ARG A 430      29.598  15.411  63.653  1.00 36.38           C
ANISOU  231  CG  ARG A 430     4689   4417   4717    -66     67     60       C
ATOM    232  CD  ARG A 430      30.321  14.483  62.727  1.00 38.04           C
ANISOU  232  CD  ARG A 430     4850   4705   4899    -11     74    -69       C
ATOM    233  NE  ARG A 430      31.735  14.848  62.498  1.00 39.38           N
ANISOU  233  NE  ARG A 430     4877   4985   5100    -56     98    -43       N
ATOM    234  CZ  ARG A 430      32.449  13.997  61.741  1.00 41.34           C
ANISOU  234  CZ  ARG A 430     5178   5209   5320     50    112   -127       C
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ATOM    235  NH1 ARG A 430      31.839  12.904  61.272  1.00 41.92           N
ANISOU  235  NH1 ARG A 430    5264   5295   5370     -5     26   -123       N
ATOM    236  NH2 ARG A 430      33.718  14.264  61.478  1.00 41.05           N
ANISOU  236  NH2 ARG A 430    5153   5243   5199     57     78   -178       N
ATOM    237  N   ASP A 431      26.427  15.931  62.583  1.00 32.85           N
ANISOU  237  N   ASP A 431    4151   4003   4327     43     10   -140       N
ATOM    238  CA  ASP A 431      25.164  15.664  63.275  1.00 33.72           C
ANISOU  238  CA  ASP A 431    4150   4041   4621     80     10    -74       C
ATOM    239  C   ASP A 431      24.129  16.766  63.080  1.00 31.60           C
ANISOU  239  C   ASP A 431    3857   4027   4123    -22    -44    -66       C
ATOM    240  O   ASP A 431      23.332  16.998  63.995  1.00 30.44           O
ANISOU  240  O   ASP A 431    3767   3721   4077     55   -132    -77       O
ATOM    241  CB  ASP A 431      25.525  15.576  64.761  1.00 37.31           C
ANISOU  241  CB  ASP A 431    4767   4659   4751    114   -111    -60       C
ATOM    242  CG  ASP A 431      24.609  14.787  65.650  1.00 41.39           C
ANISOU  242  CG  ASP A 431    5255   5147   5323    -76     98     70       C
ATOM    243  OD1 ASP A 431      23.647  14.173  65.134  1.00 42.79           O
ANISOU  243  OD1 ASP A 431    5319   5455   5483    -86    -56      5       O
ATOM    244  OD2 ASP A 431      24.864  14.779  66.885  1.00 43.70           O
ANISOU  244  OD2 ASP A 431    5720   5403   5480    -44   -113     12       O
ATOM    245  N   ASN A 432      24.144  17.410  61.939  1.00 29.57           N
ANISOU  245  N   ASN A 432    3550   3664   4020     14    -83   -160       N
ATOM    246  CA  ASN A 432      23.245  18.491  61.558  1.00 30.19           C
ANISOU  246  CA  ASN A 432    3732   3756   3981     62    -93   -159       C
ATOM    247  C   ASN A 432      23.346  19.756  62.389  1.00 28.16           C
ANISOU  247  C   ASN A 432    3365   3547   3789     81    -36    -40       C
ATOM    248  O   ASN A 432      22.390  20.483  62.639  1.00 25.96           O
ANISOU  248  O   ASN A 432    2946   3382   3537   -156   -248    -88       O
ATOM    249  CB  ASN A 432      21.786  18.014  61.397  1.00 31.82           C
ANISOU  249  CB  ASN A 432    3892   4041   4158    -62   -136   -102       C
ATOM    250  CG  ASN A 432      21.481  18.031  59.900  1.00 33.21           C
ANISOU  250  CG  ASN A 432    4242   4239   4136     44    -48    -67       C
ATOM    251  OD1 ASN A 432      21.410  16.952  59.304  1.00 34.07           O
ANISOU  251  OD1 ASN A 432    4423   4318   4204     96   -199   -152       O
ATOM    252  ND2 ASN A 432      21.340  19.228  59.338  1.00 33.00           N
ANISOU  252  ND2 ASN A 432    4252   4154   4133    101    -12   -187       N
ATOM    253  N   ILE A 433      24.579  20.075  62.807  1.00 27.29           N
ANISOU  253  N   ILE A 433    3423   3473   3472     62      3   -139       N
ATOM    254  CA  ILE A 433      24.836  21.341  63.502  1.00 27.53           C
ANISOU  254  CA  ILE A 433    3519   3359   3584    -38   -108      -2       C
ATOM    255  C   ILE A 433      26.138  21.837  62.872  1.00 27.63           C
ANISOU  255  C   ILE A 433    3655   3447   3396    -19    -33   -148       C
ATOM    256  O   ILE A 433      27.191  21.213  62.932  1.00 28.12           O
ANISOU  256  O   ILE A 433    3583   3550   3550    -70     40    -79       O
ATOM    257  CB  ILE A 433      24.851  21.252  65.009  1.00 28.90           C
ANISOU  257  CB  ILE A 433    3705   3647   3628      7      6   -121       C
ATOM    258  CG1 ILE A 433      25.119  22.600  65.684  1.00 29.59           C
ANISOU  258  CG1 ILE A 433    3759   3694   3791    -63    -86    -98       C
ATOM    259  CG2 ILE A 433      25.868  20.240  65.532  1.00 30.05           C
ANISOU  259  CG2 ILE A 433    3842   3855   3721     57    -44    -70       C
ATOM    260  CD1 ILE A 433      24.084  23.673  65.541  1.00 29.82           C
ANISOU  260  CD1 ILE A 433    3808   3683   3840    -39     12   -113       C
ATOM    261  N   GLU A 434      25.969  22.950  62.193  1.00 26.98           N
ANISOU  261  N   GLU A 434    3817   3461   2975    -28    -36   -222       N
ATOM    262  CA  GLU A 434      27.087  23.636  61.549  1.00 29.04           C
ANISOU  262  CA  GLU A 434    3782   3621   3630    -73     -4   -186       C
ATOM    263  C   GLU A 434      27.496  24.805  62.448  1.00 26.87           C
ANISOU  263  C   GLU A 434    3410   3498   3302     66    -10   -121       C
ATOM    264  O   GLU A 434      26.605  25.529  62.918  1.00 25.79           O
ANISOU  264  O   GLU A 434    3384   3312   3102      1   -171   -307       O
ATOM    265  CB  GLU A 434      26.555  24.135  60.208  1.00 32.25           C
ANISOU  265  CB  GLU A 434    4288   4141   3824     16   -151   -100       C
ATOM    266  CG  GLU A 434      27.504  25.003  59.425  1.00 35.93           C
ANISOU  266  CG  GLU A 434    4594   4572   4486   -111    112      6       C
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ATOM    267  CD  GLU A 434      26.879  25.554  58.153  1.00 38.19           C
ANISOU  267  CD  GLU A 434    4868   4933   4709     16    -31     89       C
ATOM    268  OE1 GLU A 434      25.651  25.820  58.096  1.00 39.69           O
ANISOU  268  OE1 GLU A 434    4945   5113   5020     63    136    109       O
ATOM    269  OE2 GLU A 434      27.647  25.674  57.183  1.00 39.34           O
ANISOU  269  OE2 GLU A 434    4893   5161   4894      4     80    176       O
ATOM    270  N   ILE A 435      28.784  24.958  62.728  1.00 24.78           N
ANISOU  270  N   ILE A 435    3317   3072   3025    -85    114   -224       N
ATOM    271  CA  ILE A 435      29.257  26.019  63.625  1.00 24.58           C
ANISOU  271  CA  ILE A 435    3236   3053   3049    -50     69   -179       C
ATOM    272  C   ILE A 435      30.294  26.872  62.886  1.00 24.98           C
ANISOU  272  C   ILE A 435    3223   3170   3098   -118    -12   -130       C
ATOM    273  O   ILE A 435      31.274  26.306  62.400  1.00 26.66           O
ANISOU  273  O   ILE A 435    3488   3317   3325    -43     95   -112       O
ATOM    274  CB  ILE A 435      29.821  25.456  64.940  1.00 24.87           C
ANISOU  274  CB  ILE A 435    3248   3087   3116      1     59   -187       C
ATOM    275  CG1 ILE A 435      28.785  24.576  65.663  1.00 25.95           C
ANISOU  275  CG1 ILE A 435    3476   3188   3195   -106    -43    -67       C
ATOM    276  CG2 ILE A 435      30.276  26.587  65.861  1.00 24.85           C
ANISOU  276  CG2 ILE A 435    3244   3188   3010      1    104   -180       C
ATOM    277  CD1 ILE A 435      29.256  23.840  66.869  1.00 26.22           C
ANISOU  277  CD1 ILE A 435    3513   3250   3198    -70     21     -6       C
ATOM    278  N   THR A 436      29.988  28.169  62.768  1.00 24.37           N
ANISOU  278  N   THR A 436    3273   3094   2894   -150    114     -28       N
ATOM    279  CA  THR A 436      30.940  29.080  62.136  1.00 25.67           C
ANISOU  279  CA  THR A 436    3541   3121   3091   -174     92       2       C
ATOM    280  C   THR A 436      31.724  29.829  63.189  1.00 25.18           C
ANISOU  280  C   THR A 436    3136   3245   3187   -221    131      93       C
ATOM    281  O   THR A 436      31.430  29.739  64.379  1.00 24.31           O
ANISOU  281  O   THR A 436    3137   2996   3103   -181     80    105       O
ATOM    282  CB  THR A 436      30.201  30.153  61.300  1.00 27.65           C
ANISOU  282  CB  THR A 436    3643   3418   3444    -45    -68    111       C
ATOM    283  OG1 THR A 436      29.412  31.009  62.123  1.00 27.54           O
ANISOU  283  OG1 THR A 436    3778   3251   3436   -120      6    203       O
ATOM    284  CG2 THR A 436      29.291  29.450  60.283  1.00 28.64           C
ANISOU  284  CG2 THR A 436    3783   3630   3468    -86   -130    107       C
ATOM    285  N   VAL A 437      32.736  30.592  62.713  1.00 25.05           N
ANISOU  285  N   VAL A 437    3417   2954   3148   -222    220     85       N
ATOM    286  CA  VAL A 437      33.495  31.412  63.651  1.00 24.74           C
ANISOU  286  CA  VAL A 437    3024   3161   3215   -268    253    135       C
ATOM    287  C   VAL A 437      32.579  32.414  64.333  1.00 24.55           C
ANISOU  287  C   VAL A 437    3136   3094   3096   -223    155    111       C
ATOM    288  O   VAL A 437      32.779  32.653  65.524  1.00 23.46           O
ANISOU  288  O   VAL A 437    3069   2771   3072   -143    210     83       O
ATOM    289  CB  VAL A 437      34.603  32.190  62.859  1.00 26.10           C
ANISOU  289  CB  VAL A 437    3277   3382   3258   -330    349    167       C
ATOM    290  CG1 VAL A 437      35.277  33.207  63.743  1.00 26.57           C
ANISOU  290  CG1 VAL A 437    3524   3348   3223   -185    313     65       C
ATOM    291  CG2 VAL A 437      35.602  31.101  62.489  1.00 28.12           C
ANISOU  291  CG2 VAL A 437    3345   3737   3603   -156    334     86       C
ATOM    292  N   ARG A 438      31.613  32.996  63.616  1.00 24.20           N
ANISOU  292  N   ARG A 438    3218   2981   2995   -163    220    160       N
ATOM    293  CA  ARG A 438      30.692  33.944  64.248  1.00 24.68           C
ANISOU  293  CA  ARG A 438    3290   3086   3002   -131    223    156       C
ATOM    294  C   ARG A 438      29.978  33.277  65.434  1.00 23.38           C
ANISOU  294  C   ARG A 438    3311   2812   2762    -89    125     87       C
ATOM    295  O   ARG A 438      29.904  33.861  66.514  1.00 22.44           O
ANISOU  295  O   ARG A 438    3346   2506   2675   -183    378    190       O
ATOM    296  CB  ARG A 438      29.669  34.411  63.207  1.00 28.16           C
ANISOU  296  CB  ARG A 438    3611   3594   3495    -64    -42    294       C
ATOM    297  CG  ARG A 438      28.713  35.451  63.723  1.00 31.14           C
ANISOU  297  CG  ARG A 438    4077   3779   3976     -1    157     63       C
ATOM    298  CD  ARG A 438      27.764  35.933  62.618  1.00 34.29           C
ANISOU  298  CD  ARG A 438    4372   4392   4265    -53    -72    187       C
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ATOM	299	NE	ARG	A	438	26.851	36.917	63.189	1.00	37.27			N
ANISOU	299	NE	ARG	A	438	4736	4647	4778	78	86	68		N
ATOM	300	CZ	ARG	A	438	25.791	36.661	63.952	1.00	38.91			C
ANISOU	300	CZ	ARG	A	438	4806	4921	5057	-41	97	76		C
ATOM	301	NH1	ARG	A	438	25.458	35.414	64.240	1.00	39.55			N
ANISOU	301	NH1	ARG	A	438	4980	4877	5171	-4	108	66		N
ATOM	302	NH2	ARG	A	438	25.045	37.650	64.444	1.00	39.77			N
ANISOU	302	NH2	ARG	A	438	4958	4962	5191	-40	97	-21		N
ATOM	303	N	ASP	A	439	29.495	32.063	65.276	1.00	20.60			N
ANISOU	303	N	ASP	A	439	2708	2801	2319	-32	66	39		N
ATOM	304	CA	ASP	A	439	28.883	31.366	66.411	1.00	21.02			C
ANISOU	304	CA	ASP	A	439	2826	2641	2521	-82	66	72		C
ATOM	305	C	ASP	A	439	29.881	31.095	67.540	1.00	20.11			C
ANISOU	305	C	ASP	A	439	2514	2517	2609	4	88	-1		C
ATOM	306	O	ASP	A	439	29.634	31.277	68.721	1.00	19.64			O
ANISOU	306	O	ASP	A	439	2660	2230	2572	-3	154	26		O
ATOM	307	CB	ASP	A	439	28.402	29.981	65.963	1.00	20.69			C
ANISOU	307	CB	ASP	A	439	2678	2756	2427	-199	128	-20		C
ATOM	308	CG	ASP	A	439	27.382	30.072	64.866	1.00	20.88			C
ANISOU	308	CG	ASP	A	439	2724	2697	2511	-96	144	102		C
ATOM	309	OD1	ASP	A	439	26.366	30.761	65.013	1.00	21.12			O
ANISOU	309	OD1	ASP	A	439	2808	2896	2320	41	-29	6		O
ATOM	310	OD2	ASP	A	439	27.556	29.433	63.810	1.00	23.27			O
ANISOU	310	OD2	ASP	A	439	3051	3241	2551	-67	10	-162		O
ATOM	311	N	PHE	A	440	31.076	30.603	67.161	1.00	19.54			N
ANISOU	311	N	PHE	A	440	2493	2361	2571	85	43	78		N
ATOM	312	CA	PHE	A	440	32.100	30.246	68.128	1.00	19.79			C
ANISOU	312	CA	PHE	A	440	2425	2592	2502	26	67	-134		C
ATOM	313	C	PHE	A	440	32.518	31.417	68.988	1.00	19.93			C
ANISOU	313	C	PHE	A	440	2593	2616	2365	10	-47	-24		C
ATOM	314	O	PHE	A	440	32.755	31.232	70.186	1.00	18.54			O
ANISOU	314	O	PHE	A	440	2415	2488	2140	3	225	1		O
ATOM	315	CB	PHE	A	440	33.298	29.737	67.297	1.00	19.80			C
ANISOU	315	CB	PHE	A	440	2304	2693	2526	145	190	-16		C
ATOM	316	CG	PHE	A	440	34.412	29.109	68.102	1.00	19.76			C
ANISOU	316	CG	PHE	A	440	2443	2654	2409	38	102	-108		C
ATOM	317	CD1	PHE	A	440	34.295	27.791	68.493	1.00	20.57			C
ANISOU	317	CD1	PHE	A	440	2658	2707	2451	20	81	-146		C
ATOM	318	CD2	PHE	A	440	35.575	29.780	68.471	1.00	20.34			C
ANISOU	318	CD2	PHE	A	440	2594	2644	2492	-44	137	-151		C
ATOM	319	CE1	PHE	A	440	35.257	27.125	69.211	1.00	19.74			C
ANISOU	319	CE1	PHE	A	440	2616	2507	2375	21	98	-183		C
ATOM	320	CE2	PHE	A	440	36.562	29.155	69.213	1.00	20.51			C
ANISOU	320	CE2	PHE	A	440	2598	2731	2464	12	133	-146		C
ATOM	321	CZ	PHE	A	440	36.390	27.834	69.569	1.00	20.48			C
ANISOU	321	CZ	PHE	A	440	2429	2757	2594	95	43	-26		C
ATOM	322	N	LYS	A	441	32.564	32.610	68.418	1.00	19.50			N
ANISOU	322	N	LYS	A	441	2444	2481	2483	50	21	-45		N
ATOM	323	CA	LYS	A	441	32.969	33.788	69.187	1.00	21.01			C
ANISOU	323	CA	LYS	A	441	2695	2660	2628	-30	16	-109		C
ATOM	324	C	LYS	A	441	31.985	34.146	70.277	1.00	20.16			C
ANISOU	324	C	LYS	A	441	2600	2481	2578	-113	34	-23		C
ATOM	325	O	LYS	A	441	32.310	34.937	71.190	1.00	20.20			O
ANISOU	325	O	LYS	A	441	2843	2418	2416	-5	-152	166		O
ATOM	326	CB	LYS	A	441	33.190	34.975	68.233	1.00	23.03			C
ANISOU	326	CB	LYS	A	441	3250	2780	2721	-106	9	-41		C
ATOM	327	CG	LYS	A	441	34.500	34.788	67.425	1.00	26.36			C
ANISOU	327	CG	LYS	A	441	3129	3556	3331	-82	24	-118		C
ATOM	328	CD	LYS	A	441	34.588	36.012	66.540	1.00	30.45			C
ANISOU	328	CD	LYS	A	441	4080	3816	3675	-46	-53	102		C
ATOM	329	CE	LYS	A	441	35.842	36.256	65.744	1.00	33.52			C
ANISOU	329	CE	LYS	A	441	4141	4332	4262	19	58	49		C
ATOM	330	NZ	LYS	A	441	35.868	37.745	65.450	1.00	35.91			N
ANISOU	330	NZ	LYS	A	441	4740	4423	4480	-115	13	200		N

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ATOM    331  N   THR A 442      30.747  33.575  70.269  1.00 18.17           N
ANISOU  331  N   THR A 442    2284   2270   2351    137    149    -65       N
ATOM    332  CA  THR A 442      29.833  33.861  71.383  1.00 17.18           C
ANISOU  332  CA  THR A 442    2409   1884   2237     18    106   -101       C
ATOM    333  C   THR A 442      30.334  33.146  72.634  1.00 16.91           C
ANISOU  333  C   THR A 442    2248   1942   2236    -42    130    -14       C
ATOM    334  O   THR A 442      29.800  33.382  73.738  1.00 17.17           O
ANISOU  334  O   THR A 442    2627   1783   2114    -60    151     53       O
ATOM    335  CB  THR A 442      28.360  33.521  71.114  1.00 16.82           C
ANISOU  335  CB  THR A 442    2340   1792   2258     59      8      6       C
ATOM    336  OG1 THR A 442      28.140  32.089  71.013  1.00 17.59           O
ANISOU  336  OG1 THR A 442    2466   1836   2382    -53    121    189       O
ATOM    337  CG2 THR A 442      27.887  34.234  69.832  1.00 18.39           C
ANISOU  337  CG2 THR A 442    2507   2362   2116    -31    117     96       C
ATOM    338  N   LEU A 443      31.319  32.255  72.548  1.00 16.60           N
ANISOU  338  N   LEU A 443    2351   1803   2154    -60     30     -2       N
ATOM    339  CA  LEU A 443      31.910  31.625  73.715  1.00 17.07           C
ANISOU  339  CA  LEU A 443    2333   1914   2240    -32    -87     -1       C
ATOM    340  C   LEU A 443      33.094  32.445  74.273  1.00 17.58           C
ANISOU  340  C   LEU A 443    2376   2064   2239   -107     -4    -12       C
ATOM    341  O   LEU A 443      33.661  32.059  75.292  1.00 17.55           O
ANISOU  341  O   LEU A 443    2259   2037   2371   -152    -66    -82       O
ATOM    342  CB  LEU A 443      32.463  30.205  73.358  1.00 16.65           C
ANISOU  342  CB  LEU A 443    2336   1860   2131    -40   -109     52       C
ATOM    343  CG  LEU A 443      31.329  29.177  73.206  1.00 15.42           C
ANISOU  343  CG  LEU A 443    2151   1866   1839     74    -50    -14       C
ATOM    344  CD1 LEU A 443      31.840  27.988  72.401  1.00 16.51           C
ANISOU  344  CD1 LEU A 443    2345   1676   2250     -2    -58   -104       C
ATOM    345  CD2 LEU A 443      30.799  28.717  74.570  1.00 17.06           C
ANISOU  345  CD2 LEU A 443    2415   2020   2046   -251     29     65       C
ATOM    346  N   ALA A 444      33.470  33.527  73.598  1.00 17.62           N
ANISOU  346  N   ALA A 444    2326   1928   2440    -68     21    -85       N
ATOM    347  CA  ALA A 444      34.556  34.360  74.105  1.00 17.07           C
ANISOU  347  CA  ALA A 444    2325   1896   2263     -9      0    -52       C
ATOM    348  C   ALA A 444      34.158  34.904  75.463  1.00 17.32           C
ANISOU  348  C   ALA A 444    2281   1987   2313    -64    -11   -174       C
ATOM    349  O   ALA A 444      32.971  34.984  75.854  1.00 16.91           O
ANISOU  349  O   ALA A 444    2223   1714   2488   -248     67   -154       O
ATOM    350  CB  ALA A 444      34.842  35.452  73.087  1.00 17.28           C
ANISOU  350  CB  ALA A 444    2179   2112   2272   -272    109    -37       C
ATOM    351  N   PRO A 445      35.137  35.368  76.250  1.00 16.22           N
ANISOU  351  N   PRO A 445    2052   1897   2214   -188    107   -128       N
ATOM    352  CA  PRO A 445      34.786  35.874  77.559  1.00 15.65           C
ANISOU  352  CA  PRO A 445    1914   1784   2246   -142     45   -105       C
ATOM    353  C   PRO A 445      33.720  36.952  77.505  1.00 16.92           C
ANISOU  353  C   PRO A 445    2006   2087   2335    -85     70    -74       C
ATOM    354  O   PRO A 445      33.726  37.891  76.691  1.00 17.87           O
ANISOU  354  O   PRO A 445    2256   1821   2715    -64     76   -100       O
ATOM    355  CB  PRO A 445      36.135  36.426  78.076  1.00 18.07           C
ANISOU  355  CB  PRO A 445    1973   2091   2802   -181   -144   -249       C
ATOM    356  CG  PRO A 445      37.154  35.585  77.372  1.00 20.04           C
ANISOU  356  CG  PRO A 445    2378   2661   2575     15     -1   -296       C
ATOM    357  CD  PRO A 445      36.592  35.356  75.986  1.00 19.05           C
ANISOU  357  CD  PRO A 445    2010   2515   2712   -155   -149   -187       C
ATOM    358  N   ARG A 446      32.799  36.895  78.445  1.00 16.51           N
ANISOU  358  N   ARG A 446    1952   1954   2367   -169     51    -34       N
ATOM    359  CA  ARG A 446      31.738  37.892  78.659  1.00 16.52           C
ANISOU  359  CA  ARG A 446    2082   1884   2312    -18     31      3       C
ATOM    360  C   ARG A 446      30.707  37.967  77.542  1.00 18.18           C
ANISOU  360  C   ARG A 446    2455   2151   2302      3    -50    -38       C
ATOM    361  O   ARG A 446      29.800  38.854  77.560  1.00 19.83           O
ANISOU  361  O   ARG A 446    2447   2435   2653    322     95   -144       O
ATOM    362  CB  ARG A 446      32.354  39.302  78.904  1.00 18.67           C
ANISOU  362  CB  ARG A 446    2584   1873   2638    -46   -139    -11       C
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ATOM    363  CG  ARG A 446      33.233  39.352  80.164  1.00 19.18           C
ANISOU  363  CG  ARG A 446    2624   2013   2649   -256    -95    136       C
ATOM    364  CD  ARG A 446      33.825  40.761  80.413  1.00 21.48           C
ANISOU  364  CD  ARG A 446    3307   1870   2983   -217    112    -27       C
ATOM    365  NE  ARG A 446      34.445  40.745  81.772  1.00 24.17           N
ANISOU  365  NE  ARG A 446    3506   2312   3366   -393    -36    -98       N
ATOM    366  CZ  ARG A 446      33.579  41.237  82.720  1.00 26.50           C
ANISOU  366  CZ  ARG A 446    3650   2911   3507   -271    109   -165       C
ATOM    367  NH1 ARG A 446      32.341  41.809  82.594  1.00 27.49           N
ANISOU  367  NH1 ARG A 446    3540   3097   3809   -527     31    -60       N
ATOM    368  NH2 ARG A 446      34.141  41.150  83.892  1.00 27.19           N
ANISOU  368  NH2 ARG A 446    3631   3046   3654    -92    132    179       N
ATOM    369  N   ARG A 447      30.739  37.078  76.546  1.00 17.24           N
ANISOU  369  N   ARG A 447    2395   1882   2274   -133     42     56       N
ATOM    370  CA  ARG A 447      29.759  37.166  75.475  1.00 17.00           C
ANISOU  370  CA  ARG A 447    2288   1975   2197     20     89     44       C
ATOM    371  C   ARG A 447      28.527  36.318  75.630  1.00 17.43           C
ANISOU  371  C   ARG A 447    2509   1923   2191    -78    -31    138       C
ATOM    372  O   ARG A 447      28.527  35.277  76.306  1.00 17.13           O
ANISOU  372  O   ARG A 447    2492   1791   2225    -80     98    190       O
ATOM    373  CB  ARG A 447      30.422  36.761  74.134  1.00 16.08           C
ANISOU  373  CB  ARG A 447    2170   1875   2065      1     67     88       C
ATOM    374  CG  ARG A 447      31.620  37.628  73.746  1.00 19.23           C
ANISOU  374  CG  ARG A 447    2503   2150   2653   -127     85    139       C
ATOM    375  CD  ARG A 447      31.181  39.084  73.539  1.00 20.07           C
ANISOU  375  CD  ARG A 447    2568   2248   2811    -40    103    217       C
ATOM    376  NE  ARG A 447      32.400  39.818  73.119  1.00 21.14           N
ANISOU  376  NE  ARG A 447    2589   2668   2774   -259     61     -3       N
ATOM    377  CZ  ARG A 447      32.351  41.098  72.718  1.00 22.82           C
ANISOU  377  CZ  ARG A 447    3041   2717   2911   -130     36     41       C
ATOM    378  NH1 ARG A 447      31.207  41.771  72.687  1.00 23.52           N
ANISOU  378  NH1 ARG A 447    3130   2784   3022    -93    124     37       N
ATOM    379  NH2 ARG A 447      33.497  41.683  72.324  1.00 23.53           N
ANISOU  379  NH2 ARG A 447    2965   2843   3133    -91      7   -139       N
ATOM    380  N   TRP A 448      27.415  36.853  75.135  1.00 16.90           N
ANISOU  380  N   TRP A 448    2153   1985   2283     -4     82     -5       N
ATOM    381  CA  TRP A 448      26.139  36.105  75.144  1.00 16.65           C
ANISOU  381  CA  TRP A 448    2251   2000   2075     13    -11    111       C
ATOM    382  C   TRP A 448      26.161  34.924  74.171  1.00 17.62           C
ANISOU  382  C   TRP A 448    2375   1998   2321     -5     25     47       C
ATOM    383  O   TRP A 448      26.341  35.113  72.966  1.00 18.85           O
ANISOU  383  O   TRP A 448    2476   2141   2544    197    299    108       O
ATOM    384  CB  TRP A 448      25.059  37.124  74.759  1.00 16.46           C
ANISOU  384  CB  TRP A 448    2329   1818   2108     75    127     68       C
ATOM    385  CG  TRP A 448      24.692  38.108  75.831  1.00 17.23           C
ANISOU  385  CG  TRP A 448    2464   1978   2105    -35     66     36       C
ATOM    386  CD1 TRP A 448      25.421  38.548  76.901  1.00 16.52           C
ANISOU  386  CD1 TRP A 448    2378   1786   2114     14     48    126       C
ATOM    387  CD2 TRP A 448      23.428  38.829  75.843  1.00 16.62           C
ANISOU  387  CD2 TRP A 448    2343   1782   2192    -25    148    214       C
ATOM    388  NE1 TRP A 448      24.664  39.464  77.618  1.00 17.52           N
ANISOU  388  NE1 TRP A 448    2334   2051   2272     58    274    166       N
ATOM    389  CE2 TRP A 448      23.462  39.655  76.975  1.00 17.28           C
ANISOU  389  CE2 TRP A 448    2356   1877   2332     38    201    121       C
ATOM    390  CE3 TRP A 448      22.302  38.782  75.006  1.00 17.96           C
ANISOU  390  CE3 TRP A 448    2376   1876   2572     -7    122    291       C
ATOM    391  CZ2 TRP A 448      22.379  40.488  77.337  1.00 17.68           C
ANISOU  391  CZ2 TRP A 448    2372   2030   2315     84    284     81       C
ATOM    392  CZ3 TRP A 448      21.223  39.618  75.358  1.00 19.21           C
ANISOU  392  CZ3 TRP A 448    2588   2177   2535    154    134    174       C
ATOM    393  CH2 TRP A 448      21.295  40.416  76.504  1.00 19.95           C
ANISOU  393  CH2 TRP A 448    2647   2252   2683    117     76     45       C
ATOM    394  N   LEU A 449      25.823  33.707  74.664  1.00 16.41           N
ANISOU  394  N   LEU A 449    2220   1911   2103     31     72      2       N
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ATOM    395  CA  LEU A 449      25.751  32.578  73.733  1.00 16.20           C
ANISOU  395  CA  LEU A 449    2162   1714   2279    -26     51     77       C
ATOM    396  C   LEU A 449      24.570  32.754  72.780  1.00 16.48           C
ANISOU  396  C   LEU A 449    2348   1821   2094      9     65    193       C
ATOM    397  O   LEU A 449      23.498  33.282  73.158  1.00 16.82           O
ANISOU  397  O   LEU A 449    2357   1897   2138      9    191    253       O
ATOM    398  CB  LEU A 449      25.499  31.216  74.415  1.00 18.25           C
ANISOU  398  CB  LEU A 449    2484   1985   2467     45     26    309       C
ATOM    399  CG  LEU A 449      26.444  30.771  75.511  1.00 20.89           C
ANISOU  399  CG  LEU A 449    2977   2293   2668     12   -206    286       C
ATOM    400  CD1 LEU A 449      26.437  29.257  75.726  1.00 19.38           C
ANISOU  400  CD1 LEU A 449    2722   2166   2474    124    189    256       C
ATOM    401  CD2 LEU A 449      27.770  31.407  75.583  1.00 20.64           C
ANISOU  401  CD2 LEU A 449    2591   2473   2777    287      4    525       C
ATOM    402  N   ASN A 450      24.755  32.215  71.570  1.00 16.37           N
ANISOU  402  N   ASN A 450    2335   1977   1909    -97    -33    213       N
ATOM    403  CA  ASN A 450      23.617  32.195  70.626  1.00 16.97           C
ANISOU  403  CA  ASN A 450    2214   2144   2090   -234      2    149       C
ATOM    404  C   ASN A 450      23.064  30.771  70.543  1.00 17.29           C
ANISOU  404  C   ASN A 450    2329   1957   2283      3    -42     70       C
ATOM    405  O   ASN A 450      23.514  29.804  71.181  1.00 17.29           O
ANISOU  405  O   ASN A 450    2425   2156   1988   -210    103    340       O
ATOM    406  CB  ASN A 450      23.975  32.743  69.256  1.00 18.47           C
ANISOU  406  CB  ASN A 450    2545   2410   2063    -22    114    146       C
ATOM    407  CG  ASN A 450      24.845  31.821  68.444  1.00 18.73           C
ANISOU  407  CG  ASN A 450    2422   2412   2281    -13    254    238       C
ATOM    408  OD1 ASN A 450      25.269  30.731  68.840  1.00 18.52           O
ANISOU  408  OD1 ASN A 450    2358   2427   2254    -27    104    172       O
ATOM    409  ND2 ASN A 450      25.140  32.369  67.258  1.00 18.94           N
ANISOU  409  ND2 ASN A 450    2542   2653   2001    -85    151    203       N
ATOM    410  N   ASP A 451      22.010  30.650  69.740  1.00 16.71           N
ANISOU  410  N   ASP A 451    2313   2006   2029    -86     53     -7       N
ATOM    411  CA  ASP A 451      21.294  29.362  69.628  1.00 18.13           C
ANISOU  411  CA  ASP A 451    2292   2124   2473    -48     66    -59       C
ATOM    412  C   ASP A 451      22.162  28.253  69.066  1.00 18.12           C
ANISOU  412  C   ASP A 451    2461   2210   2213    -31     -7    -51       C
ATOM    413  O   ASP A 451      21.901  27.089  69.356  1.00 17.38           O
ANISOU  413  O   ASP A 451    2498   2203   1904     -9     77    111       O
ATOM    414  CB  ASP A 451      20.045  29.564  68.761  1.00 20.04           C
ANISOU  414  CB  ASP A 451    2600   2647   2367    -27    -12     58       C
ATOM    415  CG  ASP A 451      20.408  30.031  67.341  1.00 21.13           C
ANISOU  415  CG  ASP A 451    2799   2721   2507    -15     54    115       C
ATOM    416  OD1 ASP A 451      20.501  31.259  67.145  1.00 21.53           O
ANISOU  416  OD1 ASP A 451    2841   2714   2626      6     -9    133       O
ATOM    417  OD2 ASP A 451      20.625  29.148  66.500  1.00 21.94           O
ANISOU  417  OD2 ASP A 451    3021   2743   2575    -29   -103     39       O
ATOM    418  N   THR A 452      23.146  28.570  68.237  1.00 17.61           N
ANISOU  418  N   THR A 452    2184   2145   2364      9     19     -3       N
ATOM    419  CA  THR A 452      24.010  27.552  67.636  1.00 17.98           C
ANISOU  419  CA  THR A 452    2468   2252   2113    -41    144   -106       C
ATOM    420  C   THR A 452      24.854  26.844  68.653  1.00 17.29           C
ANISOU  420  C   THR A 452    2412   2199   1958    -97    242    -76       C
ATOM    421  O   THR A 452      24.979  25.617  68.675  1.00 17.49           O
ANISOU  421  O   THR A 452    2619   2167   1860     20     82   -265       O
ATOM    422  CB  THR A 452      24.927  28.219  66.582  1.00 18.78           C
ANISOU  422  CB  THR A 452    2403   2352   2379    -20    156    109       C
ATOM    423  OG1 THR A 452      24.088  29.014  65.715  1.00 21.03           O
ANISOU  423  OG1 THR A 452    2868   2760   2364    170     37    107       O
ATOM    424  CG2 THR A 452      25.681  27.149  65.829  1.00 17.83           C
ANISOU  424  CG2 THR A 452    2391   2303   2081   -118    -51     20       C
ATOM    425  N   ILE A 453      25.409  27.621  69.597  1.00 17.00           N
ANISOU  425  N   ILE A 453    2383   2146   1932    -12     39    -57       N
ATOM    426  CA  ILE A 453      26.202  27.037  70.678  1.00 16.62           C
ANISOU  426  CA  ILE A 453    2135   2182   1998   -137      3     26       C
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ATOM    427  C   ILE A 453      25.319  26.242  71.631  1.00 15.53           C
ANISOU  427  C   ILE A 453    2092   2103   1705     37     10    -45       C
ATOM    428  O   ILE A 453      25.675  25.148  72.069  1.00 16.87           O
ANISOU  428  O   ILE A 453    2307   2095   2006    -66     92      4       O
ATOM    429  CB  ILE A 453      27.012  28.127  71.415  1.00 15.67           C
ANISOU  429  CB  ILE A 453    2109   1918   1927    -84     74     52       C
ATOM    430  CG1 ILE A 453      27.941  28.842  70.404  1.00 16.39           C
ANISOU  430  CG1 ILE A 453    2156   2103   1970    -73    107    -45       C
ATOM    431  CG2 ILE A 453      27.780  27.454  72.545  1.00 16.95           C
ANISOU  431  CG2 ILE A 453    2183   2332   1923     29    -87   -101       C
ATOM    432  CD1 ILE A 453      28.868  27.950  69.578  1.00 17.17           C
ANISOU  432  CD1 ILE A 453    2361   2131   2034     31    129    -48       C
ATOM    433  N   ILE A 454      24.133  26.778  71.985  1.00 16.23           N
ANISOU  433  N   ILE A 454    2058   2309   1801     31    123   -109       N
ATOM    434  CA  ILE A 454      23.193  26.021  72.822  1.00 16.62           C
ANISOU  434  CA  ILE A 454    2283   1992   2041    -18     54    -31       C
ATOM    435  C   ILE A 454      22.830  24.702  72.114  1.00 17.03           C
ANISOU  435  C   ILE A 454    2193   2045   2234    -92     81    -41       C
ATOM    436  O   ILE A 454      22.891  23.656  72.787  1.00 16.67           O
ANISOU  436  O   ILE A 454    2264   1963   2107    -34    174   -102       O
ATOM    437  CB  ILE A 454      21.894  26.853  73.011  1.00 17.04           C
ANISOU  437  CB  ILE A 454    2153   2215   2105    -64    127      7       C
ATOM    438  CG1 ILE A 454      22.190  28.126  73.809  1.00 18.96           C
ANISOU  438  CG1 ILE A 454    2510   2180   2512    -73     22     -2       C
ATOM    439  CG2 ILE A 454      20.810  25.981  73.661  1.00 17.94           C
ANISOU  439  CG2 ILE A 454    2037   2285   2496     21    226     46       C
ATOM    440  CD1 ILE A 454      22.608  27.891  75.239  1.00 20.59           C
ANISOU  440  CD1 ILE A 454    2780   2440   2603    -43     -5    112       C
ATOM    441  N   GLU A 455      22.571  24.722  70.813  1.00 17.22           N
ANISOU  441  N   GLU A 455    2228   2031   2283    -15     31     33       N
ATOM    442  CA  GLU A 455      22.177  23.478  70.134  1.00 18.12           C
ANISOU  442  CA  GLU A 455    2238   2312   2337      3     25    -68       C
ATOM    443  C   GLU A 455      23.338  22.478  70.115  1.00 19.31           C
ANISOU  443  C   GLU A 455    2423   2399   2513    -49     -1     57       C
ATOM    444  O   GLU A 455      23.156  21.284  70.345  1.00 19.67           O
ANISOU  444  O   GLU A 455    2602   2216   2654     72    -57   -124       O
ATOM    445  CB  GLU A 455      21.698  23.761  68.713  1.00 19.41           C
ANISOU  445  CB  GLU A 455    2682   2388   2306    -73    -32    -33       C
ATOM    446  CG  GLU A 455      21.251  22.457  68.040  1.00 21.19           C
ANISOU  446  CG  GLU A 455    2963   2470   2619      3    -10   -185       C
ATOM    447  CD  GLU A 455      20.417  22.586  66.803  1.00 22.79           C
ANISOU  447  CD  GLU A 455    2987   2925   2748    -18    -34   -157       C
ATOM    448  OE1 GLU A 455      20.242  23.696  66.274  1.00 23.95           O
ANISOU  448  OE1 GLU A 455    3301   2994   2804    -97    -66   -171       O
ATOM    449  OE2 GLU A 455      19.885  21.537  66.393  1.00 23.35           O
ANISOU  449  OE2 GLU A 455    3067   3011   2796    -30   -122   -346       O
ATOM    450  N   PHE A 456      24.534  23.010  69.840  1.00 18.48           N
ANISOU  450  N   PHE A 456    2280   2217   2525     55    160   -114       N
ATOM    451  CA  PHE A 456      25.708  22.117  69.855  1.00 16.99           C
ANISOU  451  CA  PHE A 456    1926   2110   2421    -34    -87    -69       C
ATOM    452  C   PHE A 456      25.801  21.417  71.207  1.00 17.77           C
ANISOU  452  C   PHE A 456    2112   2216   2426    -75    -39    -21       C
ATOM    453  O   PHE A 456      26.034  20.189  71.267  1.00 17.72           O
ANISOU  453  O   PHE A 456    2169   2172   2390    -14    131    -59       O
ATOM    454  CB  PHE A 456      27.038  22.894  69.617  1.00 17.46           C
ANISOU  454  CB  PHE A 456    2094   1977   2561    -25    -30    -76       C
ATOM    455  CG  PHE A 456      28.233  22.020  69.912  1.00 18.81           C
ANISOU  455  CG  PHE A 456    2537   2248   2363     85      5   -103       C
ATOM    456  CD1 PHE A 456      28.627  21.018  69.041  1.00 19.99           C
ANISOU  456  CD1 PHE A 456    2549   2399   2647    164    -32   -139       C
ATOM    457  CD2 PHE A 456      28.912  22.152  71.109  1.00 17.34           C
ANISOU  457  CD2 PHE A 456    1873   2165   2550    116    -70    -27       C
ATOM    458  CE1 PHE A 456      29.701  20.207  69.339  1.00 21.78           C
ANISOU  458  CE1 PHE A 456    2865   2632   2778    152   -135    -83       C
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ATOM    459  CE2 PHE A 456      30.007  21.367  71.441  1.00 18.50           C
ANISOU  459  CE2 PHE A 456    2489   2110   2429     92     47      5       C
ATOM    460  CZ  PHE A 456      30.376  20.381  70.544  1.00 20.03           C
ANISOU  460  CZ  PHE A 456    2484   2431   2696    202     49   -140       C
ATOM    461  N   PHE A 457      25.649  22.147  72.309  1.00 17.68           N
ANISOU  461  N   PHE A 457    2221   2042   2455     22    -99    -16       N
ATOM    462  CA  PHE A 457      25.779  21.509  73.619  1.00 17.30           C
ANISOU  462  CA  PHE A 457    2163   2083   2327    -67     -8     -1       C
ATOM    463  C   PHE A 457      24.667  20.504  73.902  1.00 17.52           C
ANISOU  463  C   PHE A 457    2224   2034   2401     -6    -66   -152       C
ATOM    464  O   PHE A 457      24.959  19.421  74.436  1.00 17.26           O
ANISOU  464  O   PHE A 457    2118   2119   2319     45     -4    -80       O
ATOM    465  CB  PHE A 457      25.939  22.527  74.752  1.00 18.77           C
ANISOU  465  CB  PHE A 457    2526   2129   2476    119    -52   -120       C
ATOM    466  CG  PHE A 457      26.522  21.867  75.981  1.00 18.03           C
ANISOU  466  CG  PHE A 457    2197   2162   2490    112     25   -130       C
ATOM    467  CD1 PHE A 457      27.910  21.562  75.985  1.00 18.56           C
ANISOU  467  CD1 PHE A 457    2185   2403   2465   -149     33     29       C
ATOM    468  CD2 PHE A 457      25.743  21.538  77.054  1.00 18.50           C
ANISOU  468  CD2 PHE A 457    2685   1997   2349     14    -56    -28       C
ATOM    469  CE1 PHE A 457      28.437  20.917  77.096  1.00 17.93           C
ANISOU  469  CE1 PHE A 457    2126   2104   2582   -131    -59    -38       C
ATOM    470  CE2 PHE A 457      26.273  20.898  78.174  1.00 18.60           C
ANISOU  470  CE2 PHE A 457    2472   2173   2420    125   -115   -157       C
ATOM    471  CZ  PHE A 457      27.608  20.582  78.178  1.00 18.40           C
ANISOU  471  CZ  PHE A 457    2452   2132   2409   -240    -78   -176       C
ATOM    472  N   MET A 458      23.474  20.772  73.430  1.00 16.73           N
ANISOU  472  N   MET A 458    2215   1843   2297     87     31   -239       N
ATOM    473  CA  MET A 458      22.376  19.810  73.550  1.00 16.99           C
ANISOU  473  CA  MET A 458    2174   1730   2552     85     40   -213       C
ATOM    474  C   MET A 458      22.774  18.520  72.788  1.00 17.29           C
ANISOU  474  C   MET A 458    2150   1938   2482    100     96   -291       C
ATOM    475  O   MET A 458      22.569  17.419  73.319  1.00 19.89           O
ANISOU  475  O   MET A 458    2409   2255   2893     24    -70   -115       O
ATOM    476  CB  MET A 458      21.054  20.373  73.014  1.00 16.73           C
ANISOU  476  CB  MET A 458    2411   1892   2055    156    -29   -197       C
ATOM    477  CG  MET A 458      20.554  21.631  73.744  1.00 17.55           C
ANISOU  477  CG  MET A 458    2396   1712   2561     76    142   -111       C
ATOM    478  SD  MET A 458      20.296  21.390  75.504  1.00 17.18           S
ANISOU  478  SD  MET A 458    2306   1587   2633    -60    230    -71       S
ATOM    479  CE  MET A 458      21.743  22.189  76.188  1.00 19.31           C
ANISOU  479  CE  MET A 458    2814   2040   2482   -237     38   -208       C
ATOM    480  N   LYS A 459      23.329  18.660  71.604  1.00 17.26           N
ANISOU  480  N   LYS A 459    2356   1811   2392    186    -64   -198       N
ATOM    481  CA  LYS A 459      23.750  17.460  70.828  1.00 19.22           C
ANISOU  481  CA  LYS A 459    2632   2005   2665    152     72   -251       C
ATOM    482  C   LYS A 459      24.822  16.681  71.551  1.00 20.55           C
ANISOU  482  C   LYS A 459    2568   2368   2871     24   -100    -94       C
ATOM    483  O   LYS A 459      24.834  15.431  71.585  1.00 22.61           O
ANISOU  483  O   LYS A 459    2828   2342   3423    117    -89   -148       O
ATOM    484  CB  LYS A 459      24.269  17.893  69.449  1.00 20.32           C
ANISOU  484  CB  LYS A 459    2664   2381   2676    325    187   -201       C
ATOM    485  CG  LYS A 459      23.133  18.323  68.503  1.00 24.79           C
ANISOU  485  CG  LYS A 459    2792   3252   3376    249    -70    -17       C
ATOM    486  CD  LYS A 459      22.501  17.176  67.749  1.00 30.15           C
ANISOU  486  CD  LYS A 459    3840   3746   3871     10    -90   -200       C
ATOM    487  CE  LYS A 459      21.777  17.804  66.526  1.00 32.80           C
ANISOU  487  CE  LYS A 459    3972   4352   4140    233    -87     13       C
ATOM    488  NZ  LYS A 459      21.337  16.664  65.686  1.00 35.13           N
ANISOU  488  NZ  LYS A 459    4317   4691   4339     -1    -12   -136       N
ATOM    489  N   TYR A 460      25.790  17.411  72.123  1.00 19.93           N
ANISOU  489  N   TYR A 460    2247   2284   3042    121     13   -187       N
ATOM    490  CA  TYR A 460      26.836  16.734  72.895  1.00 19.98           C
ANISOU  490  CA  TYR A 460    2643   2222   2726     40    -57    -28       C
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ATOM    491  C   TYR A 460      26.267  15.906  74.054  1.00 20.30           C
ANISOU  491  C   TYR A 460    2451   2387   2873     96    182    -33       C
ATOM    492  O   TYR A 460      26.725  14.793  74.371  1.00 20.01           O
ANISOU  492  O   TYR A 460    2590   2152   2860     70    -39   -153       O
ATOM    493  CB  TYR A 460      27.835  17.786  73.370  1.00 18.90           C
ANISOU  493  CB  TYR A 460    2106   2345   2730     97    156   -181       C
ATOM    494  CG  TYR A 460      28.779  17.336  74.450  1.00 20.69           C
ANISOU  494  CG  TYR A 460    2703   2332   2826    -30     45      2       C
ATOM    495  CD1 TYR A 460      29.878  16.512  74.164  1.00 20.73           C
ANISOU  495  CD1 TYR A 460    2584   2306   2988    -27     70     43       C
ATOM    496  CD2 TYR A 460      28.596  17.700  75.760  1.00 20.86           C
ANISOU  496  CD2 TYR A 460    2665   2439   2824   -123     99     26       C
ATOM    497  CE1 TYR A 460      30.755  16.081  75.156  1.00 21.90           C
ANISOU  497  CE1 TYR A 460    2809   2506   3007   -192    -57     25       C
ATOM    498  CE2 TYR A 460      29.428  17.277  76.762  1.00 22.47           C
ANISOU  498  CE2 TYR A 460    2771   2720   3048    -87    -61    130       C
ATOM    499  CZ  TYR A 460      30.511  16.472  76.452  1.00 22.05           C
ANISOU  499  CZ  TYR A 460    2864   2592   2923   -153     19    149       C
ATOM    500  OH  TYR A 460      31.355  16.099  77.467  1.00 24.73           O
ANISOU  500  OH  TYR A 460    3230   3004   3162   -161   -142    321       O
ATOM    501  N   ILE A 461      25.329  16.459  74.820  1.00 19.01           N
ANISOU  501  N   ILE A 461    2697   2140   2385     54     99   -166       N
ATOM    502  CA  ILE A 461      24.677  15.743  75.910  1.00 19.87           C
ANISOU  502  CA  ILE A 461    2559   2227   2761     51    304   -134       C
ATOM    503  C   ILE A 461      23.874  14.573  75.357  1.00 20.86           C
ANISOU  503  C   ILE A 461    2656   2363   2909    -26     78    -52       C
ATOM    504  O   ILE A 461      24.009  13.468  75.890  1.00 22.24           O
ANISOU  504  O   ILE A 461    2661   2482   3309   -134    -89     96       O
ATOM    505  CB  ILE A 461      23.722  16.752  76.628  1.00 18.84           C
ANISOU  505  CB  ILE A 461    2628   2107   2425     55    265   -100       C
ATOM    506  CG1 ILE A 461      24.586  17.730  77.448  1.00 18.90           C
ANISOU  506  CG1 ILE A 461    2579   1924   2679     36    272    -37       C
ATOM    507  CG2 ILE A 461      22.790  15.936  77.513  1.00 20.87           C
ANISOU  507  CG2 ILE A 461    2770   2407   2752    -70    467   -178       C
ATOM    508  CD1 ILE A 461      25.508  17.178  78.498  1.00 20.48           C
ANISOU  508  CD1 ILE A 461    3146   2476   2160   -241     58   -364       C
ATOM    509  N   GLU A 462      23.211  14.742  74.214  1.00 21.71           N
ANISOU  509  N   GLU A 462    2891   2274   3082     88   -116   -169       N
ATOM    510  CA  GLU A 462      22.502  13.576  73.646  1.00 24.28           C
ANISOU  510  CA  GLU A 462    3130   2683   3412   -181   -213    -64       C
ATOM    511  C   GLU A 462      23.526  12.506  73.263  1.00 26.65           C
ANISOU  511  C   GLU A 462    3576   2961   3588     78   -124   -114       C
ATOM    512  O   GLU A 462      23.205  11.319  73.478  1.00 29.22           O
ANISOU  512  O   GLU A 462    3975   3011   4116      7   -214    -11       O
ATOM    513  CB  GLU A 462      21.823  13.963  72.333  1.00 25.44           C
ANISOU  513  CB  GLU A 462    3354   3083   3228    -14    -77   -138       C
ATOM    514  CG  GLU A 462      20.526  14.677  72.576  1.00 26.27           C
ANISOU  514  CG  GLU A 462    3280   3410   3290     31     59    -94       C
ATOM    515  CD  GLU A 462      19.792  15.049  71.300  1.00 26.77           C
ANISOU  515  CD  GLU A 462    3197   3557   3418     73      5   -102       C
ATOM    516  OE1 GLU A 462      20.493  15.311  70.292  1.00 28.84           O
ANISOU  516  OE1 GLU A 462    3595   3920   3444    107    100    -16       O
ATOM    517  OE2 GLU A 462      18.555  15.113  71.317  1.00 23.89           O
ANISOU  517  OE2 GLU A 462    3043   3045   2989   -182     76   -328       O
ATOM    518  N   LYS A 463      24.594  12.909  72.601  1.00 27.04           N
ANISOU  518  N   LYS A 463    3545   2988   3739    118   -161   -179       N
ATOM    519  CA  LYS A 463      25.637  11.933  72.195  1.00 30.01           C
ANISOU  519  CA  LYS A 463    3917   3383   4101    288    -71   -280       C
ATOM    520  C   LYS A 463      26.201  11.198  73.389  1.00 30.47           C
ANISOU  520  C   LYS A 463    4046   3525   4005    184    -29   -198       C
ATOM    521  O   LYS A 463      26.547  10.001  73.229  1.00 31.93           O
ANISOU  521  O   LYS A 463    4310   3516   4306    343    -65   -221       O
ATOM    522  CB  LYS A 463      26.724  12.649  71.406  1.00 32.61           C
ANISOU  522  CB  LYS A 463    4146   3926   4320    130    -15    -89       C
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ATOM    523  CG  LYS A 463      27.867  11.853  70.769  1.00 35.79           C
ANISOU  523  CG  LYS A 463    4441   4407   4751    236     97   -107       C
ATOM    524  CD  LYS A 463      27.330  11.030  69.607  1.00 38.85           C
ANISOU  524  CD  LYS A 463    4993   4924   4844     -8    -63   -111       C
ATOM    525  CE  LYS A 463      28.424  10.101  69.083  1.00 40.78           C
ANISOU  525  CE  LYS A 463    5246   5073   5175     94     60    -62       C
ATOM    526  NZ  LYS A 463      28.029   9.599  67.739  1.00 42.97           N
ANISOU  526  NZ  LYS A 463    5490   5561   5273    -22    -37    -72       N
ATOM    527  N   SER A 464      26.359  11.762  74.584  1.00 29.67           N
ANISOU  527  N   SER A 464    3934   3407   3931    284    -28   -184       N
ATOM    528  CA  SER A 464      26.973  11.055  75.698  1.00 28.97           C
ANISOU  528  CA  SER A 464    3755   3459   3792    237     56   -200       C
ATOM    529  C   SER A 464      26.113  10.521  76.816  1.00 29.16           C
ANISOU  529  C   SER A 464    3700   3427   3952     -1    -87    -65       C
ATOM    530  O   SER A 464      26.582  10.097  77.901  1.00 28.24           O
ANISOU  530  O   SER A 464    3542   3062   4126     84     26    249       O
ATOM    531  CB  SER A 464      28.026  12.035  76.245  1.00 29.78           C
ANISOU  531  CB  SER A 464    3809   3659   3848    160    -75   -132       C
ATOM    532  OG  SER A 464      27.431  13.251  76.610  1.00 29.52           O
ANISOU  532  OG  SER A 464    3868   3550   3798    152   -229     17       O
ATOM    533  N   THR A 465      24.793  10.647  76.656  1.00 28.41           N
ANISOU  533  N   THR A 465    3630   3105   4060    235    -16   -158       N
ATOM    534  CA  THR A 465      23.874  10.237  77.705  1.00 29.04           C
ANISOU  534  CA  THR A 465    3807   3263   3964     36    -79     -9       C
ATOM    535  C   THR A 465      22.765   9.367  77.113  1.00 29.92           C
ANISOU  535  C   THR A 465    3866   3459   4043      1   -105    -77       C
ATOM    536  O   THR A 465      22.110   9.745  76.147  1.00 28.27           O
ANISOU  536  O   THR A 465    3875   2943   3923   -227   -180   -218       O
ATOM    537  CB  THR A 465      23.179  11.425  78.396  1.00 28.00           C
ANISOU  537  CB  THR A 465    3390   3411   3838    -29    -62    -15       C
ATOM    538  OG1 THR A 465      24.185  12.412  78.730  1.00 28.05           O
ANISOU  538  OG1 THR A 465    3745   3194   3718   -291     24     27       O
ATOM    539  CG2 THR A 465      22.504  11.050  79.691  1.00 28.13           C
ANISOU  539  CG2 THR A 465    3513   3375   3800    -22   -136    134       C
ATOM    540  N   PRO A 466      22.593   8.217  77.761  1.00 31.12           N
ANISOU  540  N   PRO A 466    3965   3610   4251    -64    -32     -2       N
ATOM    541  CA  PRO A 466      21.580   7.290  77.300  1.00 30.49           C
ANISOU  541  CA  PRO A 466    3953   3494   4138    -32     38    -10       C
ATOM    542  C   PRO A 466      20.174   7.752  77.602  1.00 29.72           C
ANISOU  542  C   PRO A 466    3899   3308   4087    -52    -17     59       C
ATOM    543  O   PRO A 466      19.820   8.418  78.614  1.00 27.92           O
ANISOU  543  O   PRO A 466    3477   3036   4094   -178    -59    102       O
ATOM    544  CB  PRO A 466      21.950   5.982  77.999  1.00 31.51           C
ANISOU  544  CB  PRO A 466    4144   3575   4254     79    -73     22       C
ATOM    545  CG  PRO A 466      22.814   6.336  79.149  1.00 31.98           C
ANISOU  545  CG  PRO A 466    4032   3787   4330     45    -85     92       C
ATOM    546  CD  PRO A 466      23.338   7.725  78.931  1.00 31.87           C
ANISOU  546  CD  PRO A 466    4120   3768   4222     34     14     20       C
ATOM    547  N   ASN A 467      19.317   7.312  76.673  1.00 30.01           N
ANISOU  547  N   ASN A 467    4027   3329   4047    175    -47    -98       N
ATOM    548  CA  ASN A 467      17.882   7.496  76.691  1.00 29.27           C
ANISOU  548  CA  ASN A 467    3912   3172   4037     63     61   -143       C
ATOM    549  C   ASN A 467      17.543   8.988  76.884  1.00 26.77           C
ANISOU  549  C   ASN A 467    3503   3002   3667     35    184     47       C
ATOM    550  O   ASN A 467      16.652   9.284  77.688  1.00 25.43           O
ANISOU  550  O   ASN A 467    3435   2380   3849   -118    236     54       O
ATOM    551  CB  ASN A 467      17.272   6.706  77.864  1.00 31.93           C
ANISOU  551  CB  ASN A 467    4314   3582   4235   -106      8     34       C
ATOM    552  CG  ASN A 467      17.717   5.236  77.845  1.00 34.30           C
ANISOU  552  CG  ASN A 467    4708   3733   4592    -15     40      8       C
ATOM    553  OD1 ASN A 467      17.676   4.624  76.784  1.00 35.12           O
ANISOU  553  OD1 ASN A 467    4909   3598   4837   -226     62   -111       O
ATOM    554  ND2 ASN A 467      18.208   4.733  78.956  1.00 34.98           N
ANISOU  554  ND2 ASN A 467    4788   3804   4698     47     28     63       N
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ATOM    555  N   THR A 468      18.283   9.880  76.240  1.00 23.46           N
ANISOU  555  N   THR A 468    3151   2335   3429    284    -80   -151       N
ATOM    556  CA  THR A 468      18.032  11.308  76.475  1.00 22.54           C
ANISOU  556  CA  THR A 468    3109   2271   3182     51   -126    -79       C
ATOM    557  C   THR A 468      17.834  12.048  75.175  1.00 22.67           C
ANISOU  557  C   THR A 468    3012   2460   3143    121     26    -73       C
ATOM    558  O   THR A 468      18.567  11.809  74.234  1.00 24.15           O
ANISOU  558  O   THR A 468    3331   2680   3165    288    119    -17       O
ATOM    559  CB  THR A 468      19.280  11.897  77.200  1.00 24.18           C
ANISOU  559  CB  THR A 468    3173   2615   3398      5   -171   -105       C
ATOM    560  OG1 THR A 468      19.321  11.404  78.527  1.00 24.77           O
ANISOU  560  OG1 THR A 468    3365   2594   3454   -136   -157    -76       O
ATOM    561  CG2 THR A 468      19.156  13.431  77.335  1.00 25.20           C
ANISOU  561  CG2 THR A 468    3570   2608   3397     38    -89   -131       C
ATOM    562  N   VAL A 469      16.862  12.978  75.145  1.00 20.11           N
ANISOU  562  N   VAL A 469    2757   2167   2717     63   -160      1       N
ATOM    563  CA  VAL A 469      16.715  13.872  74.015  1.00 19.77           C
ANISOU  563  CA  VAL A 469    2753   2152   2605     20    -89   -120       C
ATOM    564  C   VAL A 469      16.977  15.273  74.579  1.00 18.75           C
ANISOU  564  C   VAL A 469    2545   2095   2485   -110    -69    -42       C
ATOM    565  O   VAL A 469      16.511  15.555  75.702  1.00 19.29           O
ANISOU  565  O   VAL A 469    2525   2117   2687   -104    148     -1       O
ATOM    566  CB  VAL A 469      15.315  13.826  73.386  1.00 18.35           C
ANISOU  566  CB  VAL A 469    2601   1953   2417    -51    -76     11       C
ATOM    567  CG1 VAL A 469      14.952  15.012  72.498  1.00 18.07           C
ANISOU  567  CG1 VAL A 469    2532   2076   2257     33     36     40       C
ATOM    568  CG2 VAL A 469      15.243  12.507  72.570  1.00 20.95           C
ANISOU  568  CG2 VAL A 469    3064   2204   2694    -68     20   -216       C
ATOM    569  N   ALA A 470      17.707  16.045  73.809  1.00 17.32           N
ANISOU  569  N   ALA A 470    2214   1828   2540     56      5   -187       N
ATOM    570  CA  ALA A 470      17.914  17.453  74.210  1.00 17.85           C
ANISOU  570  CA  ALA A 470    2268   1788   2725    -72     -6   -104       C
ATOM    571  C   ALA A 470      17.602  18.261  72.963  1.00 17.99           C
ANISOU  571  C   ALA A 470    2199   2066   2569     -9     -7   -162       C
ATOM    572  O   ALA A 470      18.336  18.213  71.970  1.00 20.67           O
ANISOU  572  O   ALA A 470    2565   2411   2878    174     78    105       O
ATOM    573  CB  ALA A 470      19.318  17.689  74.748  1.00 19.31           C
ANISOU  573  CB  ALA A 470    2174   2315   2847      9     93   -235       C
ATOM    574  N   PHE A 471      16.437  18.953  72.987  1.00 17.19           N
ANISOU  574  N   PHE A 471    2401   1730   2401   -122     90     57       N
ATOM    575  CA  PHE A 471      16.057  19.708  71.814  1.00 18.27           C
ANISOU  575  CA  PHE A 471    2217   2211   2515     39    -58     42       C
ATOM    576  C   PHE A 471      16.863  21.017  71.716  1.00 17.18           C
ANISOU  576  C   PHE A 471    2178   2138   2210     54    -64     60       C
ATOM    577  O   PHE A 471      17.316  21.515  72.758  1.00 18.28           O
ANISOU  577  O   PHE A 471    2178   2274   2492     28    -21   -128       O
ATOM    578  CB  PHE A 471      14.559  20.000  71.881  1.00 19.21           C
ANISOU  578  CB  PHE A 471    2311   2380   2608    106    -23    -80       C
ATOM    579  CG  PHE A 471      13.641  18.855  71.543  1.00 20.35           C
ANISOU  579  CG  PHE A 471    2629   2280   2821     61    -11    -59       C
ATOM    580  CD1 PHE A 471      12.771  18.333  72.479  1.00 21.16           C
ANISOU  580  CD1 PHE A 471    2677   2448   2917   -146      3    -85       C
ATOM    581  CD2 PHE A 471      13.685  18.342  70.245  1.00 20.43           C
ANISOU  581  CD2 PHE A 471    2617   2396   2750    -57   -183    -47       C
ATOM    582  CE1 PHE A 471      11.907  17.276  72.146  1.00 21.30           C
ANISOU  582  CE1 PHE A 471    2707   2495   2891   -177    -28    -22       C
ATOM    583  CE2 PHE A 471      12.813  17.296  69.904  1.00 21.06           C
ANISOU  583  CE2 PHE A 471    2543   2614   2844   -163   -185     56       C
ATOM    584  CZ  PHE A 471      11.963  16.779  70.860  1.00 22.63           C
ANISOU  584  CZ  PHE A 471    2965   2743   2890   -119    -27     41       C
ATOM    585  N   ASN A 472      17.049  21.556  70.513  1.00 16.38           N
ANISOU  585  N   ASN A 472    2110   1982   2133    150     90    -18       N
ATOM    586  CA  ASN A 472      17.469  22.913  70.358  1.00 17.74           C
ANISOU  586  CA  ASN A 472    2332   2070   2338     98     45    -29       C
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ATOM    587  C   ASN A 472      16.404  23.867  70.967  1.00 17.09           C
ANISOU  587  C   ASN A 472    2307   2054   2132     30     23     50       C
ATOM    588  O   ASN A 472      15.276  23.490  71.257  1.00 17.50           O
ANISOU  588  O   ASN A 472    2375   2234   2042     46    -56   -173       O
ATOM    589  CB  ASN A 472      17.796  23.224  68.913  1.00 19.19           C
ANISOU  589  CB  ASN A 472    2484   2441   2365    -38    -53     73       C
ATOM    590  CG  ASN A 472      16.619  23.180  67.945  1.00 20.81           C
ANISOU  590  CG  ASN A 472    2619   2728   2560     19   -130    -20       C
ATOM    591  OD1 ASN A 472      15.566  23.752  68.237  1.00 18.12           O
ANISOU  591  OD1 ASN A 472    2304   2445   2136    -94   -235    -89       O
ATOM    592  ND2 ASN A 472      16.854  22.512  66.807  1.00 21.41           N
ANISOU  592  ND2 ASN A 472    2935   2648   2554    -74    -82     -8       N
ATOM    593  N   SER A 473      16.766  25.165  71.034  1.00 16.78           N
ANISOU  593  N   SER A 473    2316   1952   2107    176    -76    -71       N
ATOM    594  CA  SER A 473      15.871  26.120  71.671  1.00 16.59           C
ANISOU  594  CA  SER A 473    2355   1909   2039    107    -19    -67       C
ATOM    595  C   SER A 473      14.662  26.506  70.821  1.00 17.79           C
ANISOU  595  C   SER A 473    2307   2177   2274     78    -38     65       C
ATOM    596  O   SER A 473      13.748  27.143  71.392  1.00 19.45           O
ANISOU  596  O   SER A 473    2484   2502   2403    232    -97     93       O
ATOM    597  CB  SER A 473      16.643  27.408  72.032  1.00 17.18           C
ANISOU  597  CB  SER A 473    2580   1755   2191     57    -16     40       C
ATOM    598  OG  SER A 473      17.266  27.936  70.895  1.00 19.85           O
ANISOU  598  OG  SER A 473    2623   2238   2683     40    392   -114       O
ATOM    599  N   PHE A 474      14.636  26.157  69.546  1.00 17.53           N
ANISOU  599  N   PHE A 474    2285   2065   2311    -36   -203      6       N
ATOM    600  CA  PHE A 474      13.496  26.490  68.688  1.00 18.89           C
ANISOU  600  CA  PHE A 474    2420   2359   2398    120    -76    130       C
ATOM    601  C   PHE A 474      12.321  25.582  69.025  1.00 18.64           C
ANISOU  601  C   PHE A 474    2454   2318   2310     58    -97     35       C
ATOM    602  O   PHE A 474      11.178  25.908  68.718  1.00 18.85           O
ANISOU  602  O   PHE A 474    2487   2253   2422     86    -73    114       O
ATOM    603  CB  PHE A 474      13.879  26.444  67.187  1.00 19.19           C
ANISOU  603  CB  PHE A 474    2443   2478   2371    -35     12     17       C
ATOM    604  CG  PHE A 474      14.952  27.483  66.871  1.00 19.51           C
ANISOU  604  CG  PHE A 474    2439   2540   2434     19    -11     68       C
ATOM    605  CD1 PHE A 474      16.249  27.055  66.629  1.00 19.12           C
ANISOU  605  CD1 PHE A 474    2375   2879   2009    -82    -17    110       C
ATOM    606  CD2 PHE A 474      14.648  28.842  66.851  1.00 19.28           C
ANISOU  606  CD2 PHE A 474    2511   2535   2281    -78    -37     91       C
ATOM    607  CE1 PHE A 474      17.266  27.963  66.372  1.00 20.03           C
ANISOU  607  CE1 PHE A 474    2701   2756   2152   -110   -118     93       C
ATOM    608  CE2 PHE A 474      15.666  29.780  66.589  1.00 19.86           C
ANISOU  608  CE2 PHE A 474    2670   2568   2307   -146     53    -58       C
ATOM    609  CZ  PHE A 474      16.950  29.308  66.353  1.00 20.70           C
ANISOU  609  CZ  PHE A 474    2784   2814   2266    -33     -8    -45       C
ATOM    610  N   PHE A 475      12.562  24.442  69.714  1.00 16.55           N
ANISOU  610  N   PHE A 475    2100   2232   1957   -126   -153     28       N
ATOM    611  CA  PHE A 475      11.468  23.564  70.146  1.00 18.34           C
ANISOU  611  CA  PHE A 475    2388   2210   2369    -45     55     46       C
ATOM    612  C   PHE A 475      10.565  24.335  71.115  1.00 17.97           C
ANISOU  612  C   PHE A 475    2187   2295   2344     30     35    121       C
ATOM    613  O   PHE A 475       9.345  24.419  70.846  1.00 19.98           O
ANISOU  613  O   PHE A 475    2286   2329   2977     94    121     39       O
ATOM    614  CB  PHE A 475      12.079  22.331  70.829  1.00 18.66           C
ANISOU  614  CB  PHE A 475    2354   2382   2355    -28     14    191       C
ATOM    615  CG  PHE A 475      11.044  21.462  71.505  1.00 18.46           C
ANISOU  615  CG  PHE A 475    2325   2246   2444    -47     44     54       C
ATOM    616  CD1 PHE A 475      10.398  20.479  70.778  1.00 18.82           C
ANISOU  616  CD1 PHE A 475    2371   2366   2413    -73    -75     83       C
ATOM    617  CD2 PHE A 475      10.743  21.630  72.848  1.00 17.98           C
ANISOU  617  CD2 PHE A 475    2236   2305   2292     -1   -148     64       C
ATOM    618  CE1 PHE A 475       9.431  19.690  71.409  1.00 19.74           C
ANISOU  618  CE1 PHE A 475    2476   2360   2663   -130     59     97       C
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ATOM    619  CE2 PHE A 475       9.788  20.846  73.497  1.00 18.76           C
ANISOU  619  CE2 PHE A 475    2431   2273   2422   -103   -178      8       C
ATOM    620  CZ  PHE A 475       9.122  19.856  72.746  1.00 19.61           C
ANISOU  620  CZ  PHE A 475    2451   2401   2600   -157   -176   -102       C
ATOM    621  N   TYR A 476      11.138  24.930  72.150  1.00 17.77           N
ANISOU  621  N   TYR A 476    2102   2192   2457    104    134    -19       N
ATOM    622  CA  TYR A 476      10.241  25.668  73.065  1.00 18.09           C
ANISOU  622  CA  TYR A 476    2260   2271   2341     66    -16   -168       C
ATOM    623  C   TYR A 476       9.597  26.854  72.351  1.00 19.49           C
ANISOU  623  C   TYR A 476    2159   2473   2775     29    -52     -8       C
ATOM    624  O   TYR A 476       8.405  27.135  72.620  1.00 19.77           O
ANISOU  624  O   TYR A 476    2355   2259   2899     66   -113   -111       O
ATOM    625  CB  TYR A 476      10.971  26.011  74.409  1.00 18.95           C
ANISOU  625  CB  TYR A 476    2243   2519   2438    -63   -169    -63       C
ATOM    626  CG  TYR A 476       9.879  26.577  75.298  1.00 19.83           C
ANISOU  626  CG  TYR A 476    2111   2665   2760     40   -156    -62       C
ATOM    627  CD1 TYR A 476       8.936  25.709  75.867  1.00 22.22           C
ANISOU  627  CD1 TYR A 476    2516   2642   3285     70     98    119       C
ATOM    628  CD2 TYR A 476       9.698  27.938  75.396  1.00 20.04           C
ANISOU  628  CD2 TYR A 476    2213   2657   2745     11      7   -159       C
ATOM    629  CE1 TYR A 476       7.866  26.193  76.602  1.00 24.48           C
ANISOU  629  CE1 TYR A 476    2860   3006   3436     -1    235    -49       C
ATOM    630  CE2 TYR A 476       8.589  28.431  76.118  1.00 21.46           C
ANISOU  630  CE2 TYR A 476    2086   2907   3159    164     94   -102       C
ATOM    631  CZ  TYR A 476       7.725  27.548  76.737  1.00 23.80           C
ANISOU  631  CZ  TYR A 476    2729   2939   3374    175    209     20       C
ATOM    632  OH  TYR A 476       6.631  28.072  77.419  1.00 25.08           O
ANISOU  632  OH  TYR A 476    2350   3420   3759     44    203    -33       O
ATOM    633  N   THR A 477      10.309  27.560  71.485  1.00 21.50           N
ANISOU  633  N   THR A 477    2740   2648   2781    116   -148    243       N
ATOM    634  CA  THR A 477       9.673  28.679  70.757  1.00 21.75           C
ANISOU  634  CA  THR A 477    2708   2534   3024     90   -163    172       C
ATOM    635  C   THR A 477       8.402  28.201  70.043  1.00 21.93           C
ANISOU  635  C   THR A 477    2741   2723   2869    -53    -41      4       C
ATOM    636  O   THR A 477       7.329  28.815  70.137  1.00 23.65           O
ANISOU  636  O   THR A 477    2810   2873   3303    -22    -11     57       O
ATOM    637  CB  THR A 477      10.626  29.228  69.682  1.00 23.32           C
ANISOU  637  CB  THR A 477    2839   2850   3170     37    -57    123       C
ATOM    638  OG1 THR A 477      11.813  29.668  70.370  1.00 23.83           O
ANISOU  638  OG1 THR A 477    2822   2740   3491     87   -217    280       O
ATOM    639  CG2 THR A 477       9.959  30.425  69.016  1.00 22.98           C
ANISOU  639  CG2 THR A 477    2878   2790   3064   -105   -140    161       C
ATOM    640  N   ASN A 478       8.506  27.135  69.257  1.00 19.70           N
ANISOU  640  N   ASN A 478    2369   2595   2522     63     70    184       N
ATOM    641  CA  ASN A 478       7.359  26.589  68.548  1.00 21.28           C
ANISOU  641  CA  ASN A 478    2546   2738   2802    -99     60     52       C
ATOM    642  C   ASN A 478       6.265  26.103  69.506  1.00 21.57           C
ANISOU  642  C   ASN A 478    2603   2859   2735     21     54    203       C
ATOM    643  O   ASN A 478       5.069  26.322  69.220  1.00 22.41           O
ANISOU  643  O   ASN A 478    2725   2775   3016     70    -23     82       O
ATOM    644  CB  ASN A 478       7.751  25.461  67.584  1.00 21.76           C
ANISOU  644  CB  ASN A 478    2654   2883   2733     19      3     49       C
ATOM    645  CG  ASN A 478       8.386  25.923  66.288  1.00 22.65           C
ANISOU  645  CG  ASN A 478    2684   3068   2853     11      3     66       C
ATOM    646  OD1 ASN A 478       8.519  27.114  65.995  1.00 24.82           O
ANISOU  646  OD1 ASN A 478    3036   3296   3099    -33     62    249       O
ATOM    647  ND2 ASN A 478       8.783  24.946  65.498  1.00 23.76           N
ANISOU  647  ND2 ASN A 478    2919   3399   2710     60     59     30       N
ATOM    648  N   LEU A 479       6.619  25.353  70.543  1.00 20.09           N
ANISOU  648  N   LEU A 479    2466   2627   2539    -44     36     78       N
ATOM    649  CA  LEU A 479       5.615  24.824  71.459  1.00 20.20           C
ANISOU  649  CA  LEU A 479    2473   2750   2451     72     -4    139       C
ATOM    650  C   LEU A 479       4.813  25.922  72.142  1.00 21.07           C
ANISOU  650  C   LEU A 479    2598   2650   2758    -20     96    119       C
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ATOM    651  O   LEU A 479       3.589  25.832  72.255  1.00 21.87           O
ANISOU  651  O   LEU A 479    2428   2969   2910    129   -127     72       O
ATOM    652  CB  LEU A 479       6.325  23.969  72.539  1.00 19.68           C
ANISOU  652  CB  LEU A 479    2477   2585   2416    106    133    195       C
ATOM    653  CG  LEU A 479       5.387  23.460  73.656  1.00 20.12           C
ANISOU  653  CG  LEU A 479    2334   2667   2645   -205     -7    183       C
ATOM    654  CD1 LEU A 479       4.357  22.478  73.093  1.00 21.56           C
ANISOU  654  CD1 LEU A 479    2457   2926   2810   -162   -217     14       C
ATOM    655  CD2 LEU A 479       6.287  22.769  74.684  1.00 20.67           C
ANISOU  655  CD2 LEU A 479    2472   2719   2662    -62     46    250       C
ATOM    656  N   SER A 480       5.513  26.983  72.522  1.00 20.65           N
ANISOU  656  N   SER A 480    2463   2809   2576     -4   -126     19       N
ATOM    657  CA  SER A 480       4.873  28.104  73.219  1.00 22.40           C
ANISOU  657  CA  SER A 480    2802   2749   2961     35     56     34       C
ATOM    658  C   SER A 480       4.069  28.969  72.258  1.00 23.42           C
ANISOU  658  C   SER A 480    2807   3087   3004      0    -17    116       C
ATOM    659  O   SER A 480       2.939  29.355  72.617  1.00 25.81           O
ANISOU  659  O   SER A 480    3132   3547   3126    279     16    234       O
ATOM    660  CB  SER A 480       5.912  28.907  74.021  1.00 23.15           C
ANISOU  660  CB  SER A 480    2992   2555   3251    111     26    -99       C
ATOM    661  OG  SER A 480       6.868  29.472  73.141  1.00 24.84           O
ANISOU  661  OG  SER A 480    3105   3002   3330     75    112   -142       O
ATOM    662  N   GLU A 481       4.617  29.234  71.070  1.00 23.26           N
ANISOU  662  N   GLU A 481    2875   3087   2874    -89   -131    185       N
ATOM    663  CA  GLU A 481       3.881  30.114  70.154  1.00 24.74           C
ANISOU  663  CA  GLU A 481    2990   3246   3165     96    -95    152       C
ATOM    664  C   GLU A 481       2.822  29.390  69.349  1.00 23.37           C
ANISOU  664  C   GLU A 481    2884   3117   2880    101     95    142       C
ATOM    665  O   GLU A 481       1.770  29.998  69.066  1.00 24.54           O
ANISOU  665  O   GLU A 481    2813   3507   3006    192     34    342       O
ATOM    666  CB  GLU A 481       4.922  30.825  69.221  1.00 26.78           C
ANISOU  666  CB  GLU A 481    3320   3527   3330    177    138    185       C
ATOM    667  CG  GLU A 481       5.826  31.730  70.060  1.00 31.33           C
ANISOU  667  CG  GLU A 481    3841   4016   4048     18    -36   -121       C
ATOM    668  CD  GLU A 481       6.870  32.524  69.310  1.00 35.02           C
ANISOU  668  CD  GLU A 481    4406   4453   4447    -52    162     85       C
ATOM    669  OE1 GLU A 481       6.924  32.439  68.073  1.00 36.89           O
ANISOU  669  OE1 GLU A 481    4700   4849   4465    -56    100    104       O
ATOM    670  OE2 GLU A 481       7.689  33.257  69.925  1.00 36.88           O
ANISOU  670  OE2 GLU A 481    4515   4544   4954   -156    167     25       O
ATOM    671  N   ARG A 482       3.015  28.135  68.992  1.00 21.49           N
ANISOU  671  N   ARG A 482    2570   3050   2543    209    162    258       N
ATOM    672  CA  ARG A 482       2.188  27.393  68.067  1.00 22.47           C
ANISOU  672  CA  ARG A 482    2691   3057   2789    155    134    176       C
ATOM    673  C   ARG A 482       1.696  26.055  68.572  1.00 21.74           C
ANISOU  673  C   ARG A 482    2602   2996   2663    193     83     57       C
ATOM    674  O   ARG A 482       1.110  25.246  67.875  1.00 21.16           O
ANISOU  674  O   ARG A 482    2603   3095   2343     -3    172    241       O
ATOM    675  CB  ARG A 482       2.993  27.229  66.743  1.00 25.91           C
ANISOU  675  CB  ARG A 482    3226   3567   3053    236    324     86       C
ATOM    676  CG  ARG A 482       3.148  28.523  65.918  1.00 27.55           C
ANISOU  676  CG  ARG A 482    3465   3622   3380    184    272    167       C
ATOM    677  CD  ARG A 482       4.168  28.296  64.764  1.00 29.36           C
ANISOU  677  CD  ARG A 482    3759   4020   3377    128    295    117       C
ATOM    678  NE  ARG A 482       5.495  28.540  65.280  1.00 30.60           N
ANISOU  678  NE  ARG A 482    3833   4101   3692      2    249     69       N
ATOM    679  CZ  ARG A 482       6.105  29.624  65.694  1.00 30.26           C
ANISOU  679  CZ  ARG A 482    3752   3949   3798     15    210    164       C
ATOM    680  NH1 ARG A 482       5.499  30.809  65.603  1.00 30.80           N
ANISOU  680  NH1 ARG A 482    3762   4052   3889    113    218    183       N
ATOM    681  NH2 ARG A 482       7.344  29.589  66.196  1.00 29.80           N
ANISOU  681  NH2 ARG A 482    3809   3799   3716     66    177    226       N
ATOM    682  N   GLY A 483       1.720  25.912  69.906  1.00 20.37           N
ANISOU  682  N   GLY A 483    2485   2747   2506    107    142    120       N
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ATOM	683	CA	GLY	A	483	1.152	24.726	70.561	1.00	20.78		C
ANISOU	683	CA	GLY	A	483	2327	2933	2634	-108	-108	173	C
ATOM	684	C	GLY	A	483	1.863	23.439	70.234	1.00	22.09		C
ANISOU	684	C	GLY	A	483	2734	2897	2761	-147	1	14	C
ATOM	685	O	GLY	A	483	2.899	23.333	69.552	1.00	22.34		O
ANISOU	685	O	GLY	A	483	2793	2887	2807	-203	46	297	O
ATOM	686	N	TYR	A	484	1.290	22.316	70.681	1.00	23.51		N
ANISOU	686	N	TYR	A	484	2961	3095	2877	-166	-53	258	N
ATOM	687	CA	TYR	A	484	1.840	20.996	70.398	1.00	24.18		C
ANISOU	687	CA	TYR	A	484	2831	3134	3222	-149	-42	113	C
ATOM	688	C	TYR	A	484	1.908	20.750	68.917	1.00	24.85		C
ANISOU	688	C	TYR	A	484	2920	3212	3309	-225	-22	99	C
ATOM	689	O	TYR	A	484	2.829	20.134	68.373	1.00	25.68		O
ANISOU	689	O	TYR	A	484	2912	3530	3316	-89	-136	39	O
ATOM	690	CB	TYR	A	484	0.969	19.896	71.077	1.00	25.45		C
ANISOU	690	CB	TYR	A	484	3023	3285	3364	-246	-41	232	C
ATOM	691	CG	TYR	A	484	1.446	18.538	70.621	1.00	27.57		C
ANISOU	691	CG	TYR	A	484	3399	3536	3540	-99	35	59	C
ATOM	692	CD1	TYR	A	484	2.689	18.055	71.027	1.00	27.46		C
ANISOU	692	CD1	TYR	A	484	3255	3569	3609	-96	-4	195	C
ATOM	693	CD2	TYR	A	484	0.699	17.734	69.781	1.00	28.19		C
ANISOU	693	CD2	TYR	A	484	3329	3635	3746	-150	-64	126	C
ATOM	694	CE1	TYR	A	484	3.178	16.839	70.607	1.00	29.04		C
ANISOU	694	CE1	TYR	A	484	3603	3627	3805	-125	36	71	C
ATOM	695	CE2	TYR	A	484	1.152	16.509	69.354	1.00	29.86		C
ANISOU	695	CE2	TYR	A	484	3540	3767	4040	-99	-26	4	C
ATOM	696	CZ	TYR	A	484	2.395	16.051	69.774	1.00	30.17		C
ANISOU	696	CZ	TYR	A	484	3708	3809	3945	-58	-88	31	C
ATOM	697	OH	TYR	A	484	2.837	14.836	69.323	1.00	30.19		O
ANISOU	697	OH	TYR	A	484	3605	3654	4210	-211	12	57	O
ATOM	698	N	GLN	A	485	0.949	21.296	68.161	1.00	26.04		N
ANISOU	698	N	GLN	A	485	3049	3313	3531	-57	-98	126	N
ATOM	699	CA	GLN	A	485	0.959	21.163	66.714	1.00	27.88		C
ANISOU	699	CA	GLN	A	485	3497	3519	3576	-58	-1	64	C
ATOM	700	C	GLN	A	485	2.241	21.717	66.112	1.00	27.34		C
ANISOU	700	C	GLN	A	485	3425	3395	3566	-24	-96	96	C
ATOM	701	O	GLN	A	485	2.730	21.171	65.129	1.00	28.29		O
ANISOU	701	O	GLN	A	485	3608	3557	3584	-70	-99	7	O
ATOM	702	CB	GLN	A	485	-0.295	21.813	66.109	1.00	30.16		C
ANISOU	702	CB	GLN	A	485	3685	3946	3827	126	-110	-2	C
ATOM	703	CG	GLN	A	485	-1.536	21.050	66.611	1.00	33.42		C
ANISOU	703	CG	GLN	A	485	4027	4272	4400	-94	36	76	C
ATOM	704	CD	GLN	A	485	-1.490	19.589	66.179	1.00	35.76		C
ANISOU	704	CD	GLN	A	485	4525	4429	4632	-41	-25	-53	C
ATOM	705	OE1	GLN	A	485	-1.014	19.249	65.087	1.00	36.70		O
ANISOU	705	OE1	GLN	A	485	4726	4565	4653	29	-49	-114	O
ATOM	706	NE2	GLN	A	485	-1.945	18.701	67.053	1.00	36.54		N
ANISOU	706	NE2	GLN	A	485	4660	4615	4608	-103	-63	-1	N
ATOM	707	N	GLY	A	486	2.787	22.774	66.745	1.00	25.29		N
ANISOU	707	N	GLY	A	486	3218	3107	3286	23	-103	226	N
ATOM	708	CA	GLY	A	486	4.035	23.339	66.255	1.00	25.80		C
ANISOU	708	CA	GLY	A	486	3091	3256	3458	29	-37	123	C
ATOM	709	C	GLY	A	486	5.263	22.462	66.449	1.00	24.56		C
ANISOU	709	C	GLY	A	486	2996	3126	3210	-61	-55	97	C
ATOM	710	O	GLY	A	486	6.311	22.842	65.915	1.00	24.75		O
ANISOU	710	O	GLY	A	486	2891	3203	3310	12	27	77	O
ATOM	711	N	VAL	A	487	5.225	21.402	67.254	1.00	23.02		N
ANISOU	711	N	VAL	A	487	2694	2949	3101	-149	-42	20	N
ATOM	712	CA	VAL	A	487	6.376	20.548	67.489	1.00	23.02		C
ANISOU	712	CA	VAL	A	487	3036	2745	2963	-56	-38	-108	C
ATOM	713	C	VAL	A	487	5.971	19.077	67.352	1.00	24.30		C
ANISOU	713	C	VAL	A	487	3106	2829	3300	-145	-11	69	C
ATOM	714	O	VAL	A	487	6.737	18.185	67.657	1.00	22.28		O
ANISOU	714	O	VAL	A	487	2931	2709	2825	-205	-61	-77	O

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ATOM    715  CB  VAL A 487       7.036  20.741  68.858  1.00 21.86           C
ANISOU  715  CB  VAL A 487    2751   2635   2919   -125     54    -17       C
ATOM    716  CG1 VAL A 487       7.717  22.130  68.930  1.00 21.21           C
ANISOU  716  CG1 VAL A 487    2762   2548   2751   -185    -30      6       C
ATOM    717  CG2 VAL A 487       6.036  20.636  70.021  1.00 22.10           C
ANISOU  717  CG2 VAL A 487    2802   2822   2772    -83    -18    -18       C
ATOM    718  N   ARG A 488       4.759  18.820  66.855  1.00 27.74           N
ANISOU  718  N   ARG A 488    3337   3501   3703    -78   -270      9       N
ATOM    719  CA  ARG A 488       4.289  17.434  66.723  1.00 29.32           C
ANISOU  719  CA  ARG A 488    3688   3536   3918   -122   -114    -55       C
ATOM    720  C   ARG A 488       5.226  16.489  66.009  1.00 28.52           C
ANISOU  720  C   ARG A 488    3495   3571   3769   -161   -204    -53       C
ATOM    721  O   ARG A 488       5.365  15.329  66.459  1.00 28.02           O
ANISOU  721  O   ARG A 488    3378   3467   3799     87   -222   -186       O
ATOM    722  CB  ARG A 488       2.904  17.505  66.023  1.00 33.15           C
ANISOU  722  CB  ARG A 488    3626   4398   4572     34    -98     41       C
ATOM    723  CG  ARG A 488       2.537  16.271  65.232  1.00 38.52           C
ANISOU  723  CG  ARG A 488    4835   4736   5064    -70    -20   -232       C
ATOM    724  CD  ARG A 488       1.369  16.524  64.248  1.00 42.82           C
ANISOU  724  CD  ARG A 488    5215   5562   5493    -33   -239     46       C
ATOM    725  NE  ARG A 488       1.696  15.754  63.020  1.00 46.19           N
ANISOU  725  NE  ARG A 488    5810   5958   5783    -63    -54   -152       N
ATOM    726  CZ  ARG A 488       1.607  16.346  61.822  1.00 48.42           C
ANISOU  726  CZ  ARG A 488    6177   6192   6027    -17    -51     53       C
ATOM    727  NH1 ARG A 488       1.219  17.616  61.769  1.00 49.70           N
ANISOU  727  NH1 ARG A 488    6368   6221   6292     42     -8    -18       N
ATOM    728  NH2 ARG A 488       1.897  15.709  60.691  1.00 49.12           N
ANISOU  728  NH2 ARG A 488    6200   6283   6181    -22     23    -48       N
ATOM    729  N   ARG A 489       5.914  16.910  64.963  1.00 28.24           N
ANISOU  729  N   ARG A 489    3384   3686   3658    -54   -286   -113       N
ATOM    730  CA  ARG A 489       6.774  16.105  64.133  1.00 29.05           C
ANISOU  730  CA  ARG A 489    3379   3834   3825    -80   -211   -176       C
ATOM    731  C   ARG A 489       8.214  16.032  64.629  1.00 27.47           C
ANISOU  731  C   ARG A 489    3253   3651   3533    -48    -94   -205       C
ATOM    732  O   ARG A 489       9.039  15.317  64.060  1.00 26.40           O
ANISOU  732  O   ARG A 489    3222   3615   3195   -264   -251   -483       O
ATOM    733  CB  ARG A 489       6.757  16.707  62.710  1.00 32.28           C
ANISOU  733  CB  ARG A 489    3978   4263   4024    -23    -37    -26       C
ATOM    734  CG  ARG A 489       5.345  16.801  62.100  1.00 35.16           C
ANISOU  734  CG  ARG A 489    4131   4656   4571    -37   -176    -93       C
ATOM    735  CD  ARG A 489       5.336  17.713  60.867  1.00 37.60           C
ANISOU  735  CD  ARG A 489    4691   4844   4753    -36   -179     34       C
ATOM    736  NE  ARG A 489       6.298  17.234  59.890  1.00 40.46           N
ANISOU  736  NE  ARG A 489    4958   5352   5064    -42     29    -13       N
ATOM    737  CZ  ARG A 489       6.094  16.403  58.876  1.00 42.42           C
ANISOU  737  CZ  ARG A 489    5348   5480   5290    -54      9   -115       C
ATOM    738  NH1 ARG A 489       7.131  16.072  58.109  1.00 42.34           N
ANISOU  738  NH1 ARG A 489    5279   5487   5322    -10    -25    -62       N
ATOM    739  NH2 ARG A 489       4.867  15.935  58.613  1.00 43.18           N
ANISOU  739  NH2 ARG A 489    5386   5600   5421    -90    -54    -56       N
ATOM    740  N   TRP A 490       8.549  16.775  65.688  1.00 25.78           N
ANISOU  740  N   TRP A 490    3103   3277   3416    -21    -30   -145       N
ATOM    741  CA  TRP A 490       9.951  16.828  66.092  1.00 25.12           C
ANISOU  741  CA  TRP A 490    3190   3150   3204    -55   -147   -154       C
ATOM    742  C   TRP A 490      10.515  15.572  66.725  1.00 24.49           C
ANISOU  742  C   TRP A 490    3117   3106   3082   -108   -119   -127       C
ATOM    743  O   TRP A 490      11.668  15.235  66.431  1.00 24.90           O
ANISOU  743  O   TRP A 490    3297   3120   3043    -36   -143    -88       O
ATOM    744  CB  TRP A 490      10.197  18.013  67.029  1.00 24.61           C
ANISOU  744  CB  TRP A 490    3235   2872   3245    -49    -42    -95       C
ATOM    745  CG  TRP A 490      10.090  19.363  66.378  1.00 24.58           C
ANISOU  745  CG  TRP A 490    3171   3084   3084    -60     17     67       C
ATOM    746  CD1 TRP A 490       9.189  19.829  65.478  1.00 24.10           C
ANISOU  746  CD1 TRP A 490    3049   2996   3112    -60     -5    -20       C
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ATOM    747  CD2 TRP A 490      11.014  20.449  66.620  1.00 24.01           C
ANISOU  747  CD2 TRP A 490    3192   2974   2958    -19     29    -80       C
ATOM    748  NE1 TRP A 490       9.472  21.148  65.149  1.00 24.22           N
ANISOU  748  NE1 TRP A 490    3183   3055   2964    -19    -54     88       N
ATOM    749  CE2 TRP A 490      10.580  21.538  65.830  1.00 24.33           C
ANISOU  749  CE2 TRP A 490    3162   2954   3128   -115      3    -36       C
ATOM    750  CE3 TRP A 490      12.144  20.591  67.427  1.00 24.49           C
ANISOU  750  CE3 TRP A 490    3075   3166   3065    -59     49    -46       C
ATOM    751  CZ2 TRP A 490      11.238  22.778  65.836  1.00 24.13           C
ANISOU  751  CZ2 TRP A 490    3104   2920   3145    -74    100     37       C
ATOM    752  CZ3 TRP A 490      12.825  21.798  67.400  1.00 23.93           C
ANISOU  752  CZ3 TRP A 490    3094   3066   2932    -35    205     -9       C
ATOM    753  CH2 TRP A 490      12.358  22.856  66.605  1.00 23.70           C
ANISOU  753  CH2 TRP A 490    3042   3054   2909    -55    103    -64       C
ATOM    754  N   MET A 491       9.793  14.860  67.597  1.00 24.48           N
ANISOU  754  N   MET A 491    3155   3047   3097   -162   -201   -129       N
ATOM    755  CA  MET A 491      10.357  13.667  68.207  1.00 26.74           C
ANISOU  755  CA  MET A 491    3478   3228   3454    -18    -74      0       C
ATOM    756  C   MET A 491      10.653  12.586  67.163  1.00 28.07           C
ANISOU  756  C   MET A 491    3601   3305   3761    -50     33   -111       C
ATOM    757  O   MET A 491      11.614  11.834  67.303  1.00 26.77           O
ANISOU  757  O   MET A 491    3319   3037   3817   -348   -126   -255       O
ATOM    758  CB  MET A 491       9.429  13.124  69.294  1.00 25.41           C
ANISOU  758  CB  MET A 491    3275   3010   3368    -49   -100    -95       C
ATOM    759  CG  MET A 491      10.043  11.980  70.104  1.00 25.95           C
ANISOU  759  CG  MET A 491    3372   3092   3396    -27    -95    -27       C
ATOM    760  SD  MET A 491      11.455  12.453  71.124  1.00 25.36           S
ANISOU  760  SD  MET A 491    3258   2972   3407     59    -94   -107       S
ATOM    761  CE  MET A 491      10.687  13.294  72.510  1.00 25.75           C
ANISOU  761  CE  MET A 491    3197   3275   3312    -36     20     -9       C
ATOM    762  N   LYS A 492       9.839  12.508  66.105  1.00 31.38           N
ANISOU  762  N   LYS A 492    3946   3914   4063    -27   -175    -23       N
ATOM    763  CA  LYS A 492      10.063  11.518  65.058  1.00 34.48           C
ANISOU  763  CA  LYS A 492    4505   4240   4356     -8     16   -158       C
ATOM    764  C   LYS A 492      11.440  11.700  64.441  1.00 34.42           C
ANISOU  764  C   LYS A 492    4472   4279   4326     43    -13    -61       C
ATOM    765  O   LYS A 492      12.174  10.747  64.191  1.00 33.93           O
ANISOU  765  O   LYS A 492    4582   4097   4213     37    -71   -133       O
ATOM    766  CB  LYS A 492       9.001  11.616  63.954  1.00 37.40           C
ANISOU  766  CB  LYS A 492    4704   4841   4665    -25   -125     62       C
ATOM    767  CG  LYS A 492       8.969  10.333  63.113  1.00 41.21           C
ANISOU  767  CG  LYS A 492    5382   5069   5205     28     37   -138       C
ATOM    768  CD  LYS A 492       7.731  10.344  62.218  1.00 44.18           C
ANISOU  768  CD  LYS A 492    5511   5680   5594     19   -123    -13       C
ATOM    769  CE  LYS A 492       7.872   9.308  61.102  1.00 46.40           C
ANISOU  769  CE  LYS A 492    5949   5896   5786      9    -31   -123       C
ATOM    770  NZ  LYS A 492       6.977   9.699  59.965  1.00 47.84           N
ANISOU  770  NZ  LYS A 492    6110   6125   5940     59   -106      1       N
ATOM    771  N   ARG A 493      11.844  12.964  64.234  1.00 33.46           N
ANISOU  771  N   ARG A 493    4409   4157   4149     45    -35   -176       N
ATOM    772  CA  ARG A 493      13.157  13.256  63.687  1.00 35.01           C
ANISOU  772  CA  ARG A 493    4529   4437   4336    -78     11    -97       C
ATOM    773  C   ARG A 493      14.297  12.989  64.649  1.00 33.12           C
ANISOU  773  C   ARG A 493    4315   3993   4275    -59     94    -97       C
ATOM    774  O   ARG A 493      15.469  13.097  64.253  1.00 34.76           O
ANISOU  774  O   ARG A 493    4464   4369   4376   -111    183   -161       O
ATOM    775  CB  ARG A 493      13.252  14.692  63.177  1.00 37.40           C
ANISOU  775  CB  ARG A 493    4860   4461   4889    -10     91    -48       C
ATOM    776  CG  ARG A 493      12.733  15.068  61.831  1.00 40.11           C
ANISOU  776  CG  ARG A 493    5084   5101   5054     -4     -2     82       C
ATOM    777  CD  ARG A 493      12.285  13.921  60.962  1.00 42.49           C
ANISOU  777  CD  ARG A 493    5606   5219   5321    -78     48    -68       C
ATOM    778  NE  ARG A 493      11.374  14.308  59.879  1.00 44.09           N
ANISOU  778  NE  ARG A 493    5637   5487   5629    -60    -33     75       N
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ATOM    779  CZ  ARG A 493      11.174  13.487  58.840  1.00 45.16           C
ANISOU  779  CZ  ARG A 493    5754   5683   5720    -66     14    -36       C
ATOM    780  NH1 ARG A 493      11.765  12.301  58.803  1.00 45.69           N
ANISOU  780  NH1 ARG A 493    5810   5731   5820    -30     27      0       N
ATOM    781  NH2 ARG A 493      10.375  13.850  57.855  1.00 45.80           N
ANISOU  781  NH2 ARG A 493    5841   5794   5767    -28      1    -15       N
ATOM    782  N   LYS A 494      14.037  12.627  65.898  1.00 30.68           N
ANISOU  782  N   LYS A 494    3877   3671   4110    -60    -11   -215       N
ATOM    783  CA  LYS A 494      15.024  12.243  66.879  1.00 31.03           C
ANISOU  783  CA  LYS A 494    3982   3858   3950      6     30   -127       C
ATOM    784  C   LYS A 494      15.262  10.725  66.784  1.00 33.20           C
ANISOU  784  C   LYS A 494    4309   3944   4364     45     11    -52       C
ATOM    785  O   LYS A 494      16.042  10.141  67.536  1.00 34.30           O
ANISOU  785  O   LYS A 494    4370   4226   4438     83    -76    -52       O
ATOM    786  CB  LYS A 494      14.615  12.566  68.320  1.00 28.35           C
ANISOU  786  CB  LYS A 494    3587   3381   3802     -8   -111    -12       C
ATOM    787  CG  LYS A 494      14.719  14.058  68.625  1.00 26.48           C
ANISOU  787  CG  LYS A 494    3213   3379   3469    -70    -68    -85       C
ATOM    788  CD  LYS A 494      16.175  14.538  68.707  1.00 24.91           C
ANISOU  788  CD  LYS A 494    3102   3178   3184     16    -77   -134       C
ATOM    789  CE  LYS A 494      16.185  16.052  68.896  1.00 25.48           C
ANISOU  789  CE  LYS A 494    3000   3264   3417   -109    -54    -60       C
ATOM    790  NZ  LYS A 494      17.581  16.541  69.066  1.00 24.30           N
ANISOU  790  NZ  LYS A 494    2909   2932   3393    -81     41   -214       N
ATOM    791  N   LYS A 495      14.470  10.041  65.939  1.00 34.71           N
ANISOU  791  N   LYS A 495    4460   4331   4395     17    -41   -126       N
ATOM    792  CA  LYS A 495      14.621   8.600  65.772  1.00 35.25           C
ANISOU  792  CA  LYS A 495    4594   4283   4518   -129    -65    -37       C
ATOM    793  C   LYS A 495      14.318   7.849  67.065  1.00 33.30           C
ANISOU  793  C   LYS A 495    4210   4099   4343    -37    -45   -203       C
ATOM    794  O   LYS A 495      14.968   6.844  67.371  1.00 32.25           O
ANISOU  794  O   LYS A 495    3975   3959   4320   -150    -63   -214       O
ATOM    795  CB  LYS A 495      16.011   8.147  65.344  1.00 38.76           C
ANISOU  795  CB  LYS A 495    4839   4867   5021     89      0   -105       C
ATOM    796  CG  LYS A 495      16.685   8.660  64.102  1.00 41.88           C
ANISOU  796  CG  LYS A 495    5401   5220   5291   -103    142     37       C
ATOM    797  CD  LYS A 495      15.714   8.934  62.972  1.00 44.34           C
ANISOU  797  CD  LYS A 495    5694   5558   5595      9    -73     54       C
ATOM    798  CE  LYS A 495      16.443   8.894  61.627  1.00 46.64           C
ANISOU  798  CE  LYS A 495    5994   5952   5774    -17     74      6       C
ATOM    799  NZ  LYS A 495      15.419   8.970  60.528  1.00 48.11           N
ANISOU  799  NZ  LYS A 495    6086   6212   5983     48    -60     58       N
ATOM    800  N   THR A 496      13.305   8.310  67.794  1.00 30.86           N
ANISOU  800  N   THR A 496    4027   3600   4100   -104   -105   -151       N
ATOM    801  CA  THR A 496      12.975   7.621  69.039  1.00 30.54           C
ANISOU  801  CA  THR A 496    4015   3560   4028     -9    -32   -205       C
ATOM    802  C   THR A 496      11.590   8.060  69.460  1.00 28.33           C
ANISOU  802  C   THR A 496    3828   3160   3777   -207   -145   -204       C
ATOM    803  O   THR A 496      10.925   8.770  68.700  1.00 28.76           O
ANISOU  803  O   THR A 496    3934   3185   3808   -142   -195   -243       O
ATOM    804  CB  THR A 496      14.032   7.883  70.122  1.00 31.29           C
ANISOU  804  CB  THR A 496    3984   3764   4143      6    -33   -179       C
ATOM    805  OG1 THR A 496      13.807   7.021  71.240  1.00 31.57           O
ANISOU  805  OG1 THR A 496    3995   3872   4129    147    -24   -158       O
ATOM    806  CG2 THR A 496      13.879   9.339  70.594  1.00 31.45           C
ANISOU  806  CG2 THR A 496    4191   3755   4003     42     73   -152       C
ATOM    807  N   GLN A 497      11.071   7.488  70.530  1.00 28.71           N
ANISOU  807  N   GLN A 497    3772   3324   3814    -97    -20   -204       N
ATOM    808  CA  GLN A 497       9.724   7.776  70.997  1.00 28.42           C
ANISOU  808  CA  GLN A 497    3655   3359   3782   -231    -49    -23       C
ATOM    809  C   GLN A 497       9.771   8.149  72.464  1.00 26.85           C
ANISOU  809  C   GLN A 497    3409   3009   3784   -247    -26    -31       C
ATOM    810  O   GLN A 497      10.605   7.681  73.248  1.00 27.05           O
ANISOU  810  O   GLN A 497    3493   2806   3978   -138    -91   -144       O
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ATOM	811	CB	GLN	A	497	8.806	6.534	70.829	1.00	30.38			C
ANISOU	811	CB	GLN	A	497	3907	3450	4184	-306	-41	-80		C
ATOM	812	CG	GLN	A	497	8.741	6.009	69.409	1.00	32.97			C
ANISOU	812	CG	GLN	A	497	4319	3985	4221	-210	-97	-101		C
ATOM	813	CD	GLN	A	497	9.923	5.137	69.015	1.00	34.66			C
ANISOU	813	CD	GLN	A	497	4538	4150	4481	-138	-45	-207		C
ATOM	814	OE1	GLN	A	497	10.465	4.356	69.800	1.00	36.17			O
ANISOU	814	OE1	GLN	A	497	4886	4141	4715	-122	-163	-167		O
ATOM	815	NE2	GLN	A	497	10.403	5.326	67.792	1.00	35.09			N
ANISOU	815	NE2	GLN	A	497	4753	4051	4527	-252	47	-169		N
ATOM	816	N	ILE	A	498	8.856	8.999	72.909	1.00	26.96			N
ANISOU	816	N	ILE	A	498	3376	3230	3639	-207	42	54		N
ATOM	817	CA	ILE	A	498	8.834	9.464	74.294	1.00	26.10			C
ANISOU	817	CA	ILE	A	498	3234	3081	3604	-228	-32	-44		C
ATOM	818	C	ILE	A	498	8.820	8.344	75.308	1.00	27.19			C
ANISOU	818	C	ILE	A	498	3387	3154	3788	-110	-88	42		C
ATOM	819	O	ILE	A	498	9.458	8.459	76.367	1.00	26.26			O
ANISOU	819	O	ILE	A	498	3535	2680	3762	-163	-90	-80		O
ATOM	820	CB	ILE	A	498	7.747	10.513	74.568	1.00	25.77			C
ANISOU	820	CB	ILE	A	498	3081	3285	3425	-121	-70	123		C
ATOM	821	CG1	ILE	A	498	7.970	11.181	75.925	1.00	25.46			C
ANISOU	821	CG1	ILE	A	498	3048	3008	3616	-153	-24	-8		C
ATOM	822	CG2	ILE	A	498	6.327	9.955	74.522	1.00	25.92			C
ANISOU	822	CG2	ILE	A	498	3222	3123	3502	-280	105	59		C
ATOM	823	CD1	ILE	A	498	7.278	12.526	76.083	1.00	26.13			C
ANISOU	823	CD1	ILE	A	498	3187	3171	3572	0	-129	-26		C
ATOM	824	N	ASP	A	499	8.157	7.193	75.038	1.00	28.65			N
ANISOU	824	N	ASP	A	499	3590	3265	4028	-176	-190	-141		N
ATOM	825	CA	ASP	A	499	8.173	6.129	76.050	1.00	30.82			C
ANISOU	825	CA	ASP	A	499	3931	3711	4067	-163	-107	52		C
ATOM	826	C	ASP	A	499	9.494	5.403	76.222	1.00	31.39			C
ANISOU	826	C	ASP	A	499	3956	3756	4214	-187	-95	-34		C
ATOM	827	O	ASP	A	499	9.627	4.594	77.172	1.00	31.89			O
ANISOU	827	O	ASP	A	499	4017	3673	4427	-142	-110	87		O
ATOM	828	CB	ASP	A	499	7.030	5.141	75.773	1.00	33.24			C
ANISOU	828	CB	ASP	A	499	4243	3872	4514	-317	-109	78		C
ATOM	829	CG	ASP	A	499	7.192	4.219	74.608	1.00	36.15			C
ANISOU	829	CG	ASP	A	499	4655	4509	4572	-143	-61	-89		C
ATOM	830	OD1	ASP	A	499	8.219	4.099	73.946	1.00	37.41			O
ANISOU	830	OD1	ASP	A	499	4793	4680	4742	-284	-42	-127		O
ATOM	831	OD2	ASP	A	499	6.193	3.482	74.333	1.00	38.16			O
ANISOU	831	OD2	ASP	A	499	4859	4729	4912	-246	-114	-63		O
ATOM	832	N	LYS	A	500	10.520	5.686	75.422	1.00	30.89			N
ANISOU	832	N	LYS	A	500	3981	3614	4141	-98	-87	-98		N
ATOM	833	CA	LYS	A	500	11.827	5.064	75.640	1.00	30.61			C
ANISOU	833	CA	LYS	A	500	3892	3519	4220	-198	-178	-147		C
ATOM	834	C	LYS	A	500	12.819	5.982	76.349	1.00	28.91			C
ANISOU	834	C	LYS	A	500	3781	3245	3959	-28	-94	-128		C
ATOM	835	O	LYS	A	500	13.970	5.604	76.514	1.00	28.04			O
ANISOU	835	O	LYS	A	500	3667	2835	4153	-183	-240	-304		O
ATOM	836	CB	LYS	A	500	12.373	4.629	74.254	1.00	34.11			C
ANISOU	836	CB	LYS	A	500	4305	4243	4411	90	48	-77		C
ATOM	837	CG	LYS	A	500	11.456	3.400	73.943	1.00	37.41			C
ANISOU	837	CG	LYS	A	500	4684	4600	4931	-123	-80	-94		C
ATOM	838	CD	LYS	A	500	11.785	2.652	72.688	1.00	39.98			C
ANISOU	838	CD	LYS	A	500	5091	5063	5037	54	-10	-138		C
ATOM	839	CE	LYS	A	500	10.608	1.784	72.266	1.00	41.14			C
ANISOU	839	CE	LYS	A	500	5202	5084	5345	-48	-37	-35		C
ATOM	840	NZ	LYS	A	500	9.401	2.609	71.943	1.00	41.53			N
ANISOU	840	NZ	LYS	A	500	5193	5156	5430	-56	-130	-88		N
ATOM	841	N	LEU	A	501	12.366	7.190	76.683	1.00	27.35			N
ANISOU	841	N	LEU	A	501	3592	3084	3714	-198	-184	-169		N
ATOM	842	CA	LEU	A	501	13.338	8.128	77.273	1.00	24.06			C
ANISOU	842	CA	LEU	A	501	3309	2524	3307	12	-104	44		C

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ATOM    843  C   LEU A 501      13.340   8.270  78.776  1.00 24.65           C
ANISOU  843  C   LEU A 501    3295   2748   3322    -48   -154     13       C
ATOM    844  O   LEU A 501      12.382   8.095  79.530  1.00 24.51           O
ANISOU  844  O   LEU A 501    3369   2662   3281   -328   -100   -137       O
ATOM    845  CB  LEU A 501      12.991   9.507  76.626  1.00 22.80           C
ANISOU  845  CB  LEU A 501    3188   2270   3207    -32    -74    -72       C
ATOM    846  CG  LEU A 501      13.115   9.641  75.114  1.00 23.38           C
ANISOU  846  CG  LEU A 501    3208   2415   3262     16   -170    -54       C
ATOM    847  CD1 LEU A 501      12.638  11.028  74.620  1.00 23.49           C
ANISOU  847  CD1 LEU A 501    3282   2413   3231     24   -189   -102       C
ATOM    848  CD2 LEU A 501      14.542   9.352  74.648  1.00 25.32           C
ANISOU  848  CD2 LEU A 501    3479   2848   3293    -21    121    -87       C
ATOM    849  N   ASP A 502      14.522   8.677  79.293  1.00 23.43           N
ANISOU  849  N   ASP A 502    3120   2349   3436   -144    -18     52       N
ATOM    850  CA  ASP A 502      14.654   8.980  80.712  1.00 23.57           C
ANISOU  850  CA  ASP A 502    3257   2325   3373   -127    100     39       C
ATOM    851  C   ASP A 502      14.382  10.496  80.901  1.00 22.78           C
ANISOU  851  C   ASP A 502    3137   2397   3122     63     51     35       C
ATOM    852  O   ASP A 502      13.750  10.911  81.856  1.00 21.88           O
ANISOU  852  O   ASP A 502    3058   2139   3117   -149    117    149       O
ATOM    853  CB  ASP A 502      16.075   8.708  81.193  1.00 28.57           C
ANISOU  853  CB  ASP A 502    3591   3354   3910     30   -109     48       C
ATOM    854  CG  ASP A 502      16.387   7.220  81.350  1.00 32.24           C
ANISOU  854  CG  ASP A 502    4240   3520   4489    122      5     10       C
ATOM    855  OD1 ASP A 502      15.442   6.425  81.379  1.00 33.56           O
ANISOU  855  OD1 ASP A 502    4614   3436   4700    -46     -5     86       O
ATOM    856  OD2 ASP A 502      17.583   6.891  81.441  1.00 34.47           O
ANISOU  856  OD2 ASP A 502    4372   3836   4889    111   -107     27       O
ATOM    857  N   LYS A 503      15.003  11.306  80.043  1.00 21.76           N
ANISOU  857  N   LYS A 503    2816   2231   3221     62    -61     75       N
ATOM    858  CA  LYS A 503      14.861  12.766  80.175  1.00 20.78           C
ANISOU  858  CA  LYS A 503    2871   2240   2786   -100    -77    -39       C
ATOM    859  C   LYS A 503      14.722  13.436  78.822  1.00 19.90           C
ANISOU  859  C   LYS A 503    2611   2113   2836   -163     51      4       C
ATOM    860  O   LYS A 503      15.260  12.961  77.820  1.00 19.92           O
ANISOU  860  O   LYS A 503    2563   2046   2959    -20     12    -67       O
ATOM    861  CB  LYS A 503      16.095  13.375  80.863  1.00 21.99           C
ANISOU  861  CB  LYS A 503    2829   2545   2980    -89   -107     42       C
ATOM    862  CG  LYS A 503      16.353  12.959  82.295  1.00 23.57           C
ANISOU  862  CG  LYS A 503    3179   2755   3020    -85   -174    118       C
ATOM    863  CD  LYS A 503      17.372  13.907  82.936  1.00 25.83           C
ANISOU  863  CD  LYS A 503    3183   3249   3383   -302   -178     36       C
ATOM    864  CE  LYS A 503      17.693  13.448  84.353  1.00 27.13           C
ANISOU  864  CE  LYS A 503    3477   3464   3368   -216    -19     80       C
ATOM    865  NZ  LYS A 503      18.191  12.036  84.332  1.00 28.53           N
ANISOU  865  NZ  LYS A 503    3575   3704   3560    -20    -24     19       N
ATOM    866  N   ILE A 504      14.062  14.597  78.796  1.00 19.58           N
ANISOU  866  N   ILE A 504    2452   2229   2759    -68     20    111       N
ATOM    867  CA  ILE A 504      14.024  15.466  77.619  1.00 19.71           C
ANISOU  867  CA  ILE A 504    2612   2159   2719   -139   -139     13       C
ATOM    868  C   ILE A 504      14.460  16.861  78.108  1.00 19.00           C
ANISOU  868  C   ILE A 504    2454   2130   2637   -222    126     -4       C
ATOM    869  O   ILE A 504      13.856  17.312  79.096  1.00 18.32           O
ANISOU  869  O   ILE A 504    2545   1805   2610   -267    180     13       O
ATOM    870  CB  ILE A 504      12.625  15.642  77.006  1.00 19.18           C
ANISOU  870  CB  ILE A 504    2403   2188   2698   -122   -104      3       C
ATOM    871  CG1 ILE A 504      12.186  14.292  76.412  1.00 21.05           C
ANISOU  871  CG1 ILE A 504    2649   2366   2982   -206   -150   -105       C
ATOM    872  CG2 ILE A 504      12.704  16.623  75.823  1.00 20.43           C
ANISOU  872  CG2 ILE A 504    2621   2359   2781   -105    -96     79       C
ATOM    873  CD1 ILE A 504      10.689  14.246  76.137  1.00 21.81           C
ANISOU  873  CD1 ILE A 504    2487   2600   3200    -45     35    -14       C
ATOM    874  N   PHE A 505      15.478  17.432  77.489  1.00 16.76           N
ANISOU  874  N   PHE A 505    2350   1723   2294   -112     50    121       N
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ATOM	875	CA	PHE	A	505	15.939	18.778	77.885	1.00	15.92			C
ANISOU	875	CA	PHE	A	505	1984	1899	2165	-26	-102	-79		C
ATOM	876	C	PHE	A	505	15.418	19.798	76.892	1.00	17.51			C
ANISOU	876	C	PHE	A	505	2517	1855	2282	-157	31	10		C
ATOM	877	O	PHE	A	505	15.458	19.531	75.680	1.00	18.22			O
ANISOU	877	O	PHE	A	505	2693	1810	2418	13	93	-40		O
ATOM	878	CB	PHE	A	505	17.497	18.864	77.935	1.00	15.84			C
ANISOU	878	CB	PHE	A	505	2001	1798	2218	-97	50	95		C
ATOM	879	CG	PHE	A	505	18.027	18.114	79.135	1.00	17.42			C
ANISOU	879	CG	PHE	A	505	2451	1851	2318	-81	-10	52		C
ATOM	880	CD1	PHE	A	505	18.435	16.796	78.952	1.00	18.07			C
ANISOU	880	CD1	PHE	A	505	2540	1921	2405	88	63	127		C
ATOM	881	CD2	PHE	A	505	18.180	18.693	80.378	1.00	17.14			C
ANISOU	881	CD2	PHE	A	505	2124	2146	2242	-31	127	75		C
ATOM	882	CE1	PHE	A	505	18.948	16.092	80.033	1.00	18.58			C
ANISOU	882	CE1	PHE	A	505	2396	2231	2434	-67	-149	100		C
ATOM	883	CE2	PHE	A	505	18.672	17.998	81.465	1.00	19.19			C
ANISOU	883	CE2	PHE	A	505	2488	2224	2580	85	-73	37		C
ATOM	884	CZ	PHE	A	505	19.076	16.666	81.285	1.00	19.09			C
ANISOU	884	CZ	PHE	A	505	2543	2145	2567	-38	14	-21		C
ATOM	885	N	THR	A	506	14.924	20.959	77.350	1.00	16.31			N
ANISOU	885	N	THR	A	506	1966	1857	2373	65	-100	195		N
ATOM	886	CA	THR	A	506	14.430	21.983	76.447	1.00	17.01			C
ANISOU	886	CA	THR	A	506	2326	1849	2288	-61	-134	102		C
ATOM	887	C	THR	A	506	15.000	23.342	76.863	1.00	16.40			C
ANISOU	887	C	THR	A	506	2127	1829	2274	28	-2	21		C
ATOM	888	O	THR	A	506	14.522	23.974	77.846	1.00	17.48			O
ANISOU	888	O	THR	A	506	2409	1929	2306	-19	19	23		O
ATOM	889	CB	THR	A	506	12.872	22.057	76.476	1.00	17.01			C
ANISOU	889	CB	THR	A	506	2206	1853	2404	-153	70	-69		C
ATOM	890	OG1	THR	A	506	12.431	22.374	77.820	1.00	18.67			O
ANISOU	890	OG1	THR	A	506	2514	2077	2504	-154	166	-42		O
ATOM	891	CG2	THR	A	506	12.276	20.709	76.080	1.00	18.31			C
ANISOU	891	CG2	THR	A	506	2451	1842	2664	-101	-151	-38		C
ATOM	892	N	PRO	A	507	16.086	23.783	76.275	1.00	16.35			N
ANISOU	892	N	PRO	A	507	2260	1805	2145	-18	52	-32		N
ATOM	893	CA	PRO	A	507	16.660	25.108	76.490	1.00	15.56			C
ANISOU	893	CA	PRO	A	507	1998	1800	2115	101	38	-174		C
ATOM	894	C	PRO	A	507	15.641	26.138	75.973	1.00	15.81			C
ANISOU	894	C	PRO	A	507	2151	1760	2096	-73	0	-12		C
ATOM	895	O	PRO	A	507	14.941	25.945	74.979	1.00	16.44			O
ANISOU	895	O	PRO	A	507	2347	1690	2208	58	8	190		O
ATOM	896	CB	PRO	A	507	17.963	25.133	75.657	1.00	16.57			C
ANISOU	896	CB	PRO	A	507	2099	2133	2063	-193	52	-133		C
ATOM	897	CG	PRO	A	507	17.661	24.174	74.537	1.00	16.13			C
ANISOU	897	CG	PRO	A	507	2028	1997	2102	-232	39	-127		C
ATOM	898	CD	PRO	A	507	16.795	23.082	75.166	1.00	16.06			C
ANISOU	898	CD	PRO	A	507	1964	2117	2022	-145	170	-38		C
ATOM	899	N	ILE	A	508	15.512	27.211	76.780	1.00	15.49			N
ANISOU	899	N	ILE	A	508	1821	1590	2476	207	94	21		N
ATOM	900	CA	ILE	A	508	14.492	28.241	76.501	1.00	16.06			C
ANISOU	900	CA	ILE	A	508	2189	1537	2375	146	-32	66		C
ATOM	901	C	ILE	A	508	15.104	29.627	76.342	1.00	14.76			C
ANISOU	901	C	ILE	A	508	1768	1682	2160	75	84	81		C
ATOM	902	O	ILE	A	508	15.881	30.041	77.202	1.00	16.01			O
ANISOU	902	O	ILE	A	508	2335	1501	2246	42	125	0		O
ATOM	903	CB	ILE	A	508	13.540	28.264	77.698	1.00	17.17			C
ANISOU	903	CB	ILE	A	508	1886	1924	2713	101	72	89		C
ATOM	904	CG1	ILE	A	508	12.766	26.906	77.805	1.00	18.68			C
ANISOU	904	CG1	ILE	A	508	2437	2058	2603	49	182	162		C
ATOM	905	CG2	ILE	A	508	12.512	29.416	77.577	1.00	18.32			C
ANISOU	905	CG2	ILE	A	508	2289	1951	2720	288	255	89		C
ATOM	906	CD1	ILE	A	508	12.105	26.794	79.167	1.00	21.03			C
ANISOU	906	CD1	ILE	A	508	2779	2685	2525	165	159	13		C

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ATOM	907	N	ASN	A	509	14.769	30.269	75.218	1.00	16.29		N
ANISOU	907	N	ASN	A	509	2216	1847	2125	67	11	41	N
ATOM	908	CA	ASN	A	509	15.243	31.625	74.991	1.00	16.80		C
ANISOU	908	CA	ASN	A	509	2221	1928	2234	-35	-23	-43	C
ATOM	909	C	ASN	A	509	14.106	32.539	75.453	1.00	18.14		C
ANISOU	909	C	ASN	A	509	2297	2141	2454	57	-4	-80	C
ATOM	910	O	ASN	A	509	12.941	32.250	75.139	1.00	21.01		O
ANISOU	910	O	ASN	A	509	2471	2365	3147	63	-232	-141	O
ATOM	911	CB	ASN	A	509	15.453	31.934	73.507	1.00	19.29		C
ANISOU	911	CB	ASN	A	509	2709	2328	2291	14	17	101	C
ATOM	912	CG	ASN	A	509	16.026	33.346	73.388	1.00	19.06		C
ANISOU	912	CG	ASN	A	509	2477	2244	2520	53	-147	69	C
ATOM	913	OD1	ASN	A	509	15.293	34.259	72.963	1.00	20.78		O
ANISOU	913	OD1	ASN	A	509	2749	2310	2836	182	-291	250	O
ATOM	914	ND2	ASN	A	509	17.304	33.535	73.676	1.00	18.78		N
ANISOU	914	ND2	ASN	A	509	2533	2406	2195	77	-80	262	N
ATOM	915	N	LEU	A	510	14.429	33.498	76.303	1.00	18.10		N
ANISOU	915	N	LEU	A	510	2188	2146	2542	126	-134	-165	N
ATOM	916	CA	LEU	A	510	13.405	34.404	76.826	1.00	20.12		C
ANISOU	916	CA	LEU	A	510	2447	2387	2812	150	82	-51	C
ATOM	917	C	LEU	A	510	13.677	35.792	76.249	1.00	22.23		C
ANISOU	917	C	LEU	A	510	2851	2477	3117	9	62	5	C
ATOM	918	O	LEU	A	510	14.658	36.428	76.654	1.00	21.24		O
ANISOU	918	O	LEU	A	510	2656	2501	2913	83	171	201	O
ATOM	919	CB	LEU	A	510	13.497	34.430	78.351	1.00	22.33		C
ANISOU	919	CB	LEU	A	510	2925	2691	2867	214	167	-78	C
ATOM	920	CG	LEU	A	510	13.138	33.057	78.971	1.00	25.04		C
ANISOU	920	CG	LEU	A	510	3471	2861	3181	-72	84	5	C
ATOM	921	CD1	LEU	A	510	13.746	32.940	80.370	1.00	27.03		C
ANISOU	921	CD1	LEU	A	510	3670	3299	3300	-117	-12	95	C
ATOM	922	CD2	LEU	A	510	11.649	32.824	79.011	1.00	26.25		C
ANISOU	922	CD2	LEU	A	510	3524	3043	3407	-11	8	74	C
ATOM	923	N	ASN	A	511	12.822	36.222	75.336	1.00	23.67		N
ANISOU	923	N	ASN	A	511	3078	2707	3207	14	-111	36	N
ATOM	924	CA	ASN	A	511	12.839	37.585	74.828	1.00	26.61		C
ANISOU	924	CA	ASN	A	511	3453	3017	3643	-8	51	284	C
ATOM	925	C	ASN	A	511	14.140	38.077	74.259	1.00	24.33		C
ANISOU	925	C	ASN	A	511	3173	2674	3396	111	-34	7	C
ATOM	926	O	ASN	A	511	14.493	39.265	74.368	1.00	23.65		O
ANISOU	926	O	ASN	A	511	3162	2356	3470	367	44	32	O
ATOM	927	CB	ASN	A	511	12.494	38.544	76.000	1.00	29.89		C
ANISOU	927	CB	ASN	A	511	4028	3487	3842	116	-38	62	C
ATOM	928	CG	ASN	A	511	11.173	38.196	76.663	1.00	34.64		C
ANISOU	928	CG	ASN	A	511	4283	4313	4568	-107	140	89	C
ATOM	929	OD1	ASN	A	511	10.153	38.126	75.973	1.00	36.77		O
ANISOU	929	OD1	ASN	A	511	4452	4802	4717	-42	-19	45	O
ATOM	930	ND2	ASN	A	511	11.208	37.969	77.978	1.00	37.35		N
ANISOU	930	ND2	ASN	A	511	4792	4745	4656	-83	-9	34	N
ATOM	931	N	GLN	A	512	14.927	37.179	73.659	1.00	22.30		N
ANISOU	931	N	GLN	A	512	2758	2502	3211	158	-22	256	N
ATOM	932	CA	GLN	A	512	16.230	37.545	73.105	1.00	21.51		C
ANISOU	932	CA	GLN	A	512	2922	2385	2868	126	51	214	C
ATOM	933	C	GLN	A	512	17.133	38.170	74.131	1.00	21.94		C
ANISOU	933	C	GLN	A	512	2912	2471	2953	318	0	88	C
ATOM	934	O	GLN	A	512	18.072	38.889	73.731	1.00	22.45		O
ANISOU	934	O	GLN	A	512	3027	2550	2951	175	-17	119	O
ATOM	935	CB	GLN	A	512	16.055	38.478	71.882	1.00	21.79		C
ANISOU	935	CB	GLN	A	512	3063	2399	2817	76	74	215	C
ATOM	936	CG	GLN	A	512	15.366	37.787	70.728	1.00	23.35		C
ANISOU	936	CG	GLN	A	512	3270	2775	2827	115	10	138	C
ATOM	937	CD	GLN	A	512	16.254	36.895	69.898	1.00	22.57		C
ANISOU	937	CD	GLN	A	512	2948	2714	2914	17	-43	101	C
ATOM	938	OE1	GLN	A	512	17.459	36.829	70.152	1.00	23.69		O
ANISOU	938	OE1	GLN	A	512	3046	2928	3029	403	-92	-177	O

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ATOM	939	NE2	GLN	A	512	15.721	36.260	68.873	1.00	22.83		N
ANISOU	939	NE2	GLN	A	512	3131	2652	2890	97	-267	229	N
ATOM	940	N	SER	A	513	16.947	37.863	75.424	1.00	21.26		N
ANISOU	940	N	SER	A	513	3014	2102	2963	222	-10	104	N
ATOM	941	CA	SER	A	513	17.808	38.469	76.418	1.00	22.17		C
ANISOU	941	CA	SER	A	513	2947	2470	3006	102	-75	116	C
ATOM	942	C	SER	A	513	18.251	37.509	77.507	1.00	19.87		C
ANISOU	942	C	SER	A	513	2649	2135	2768	-92	70	38	C
ATOM	943	O	SER	A	513	19.119	37.874	78.252	1.00	19.87		O
ANISOU	943	O	SER	A	513	2798	1930	2822	-10	80	291	O
ATOM	944	CB	SER	A	513	17.108	39.688	77.039	1.00	25.47		C
ANISOU	944	CB	SER	A	513	3544	2743	3392	172	69	-97	C
ATOM	945	OG	SER	A	513	16.001	39.285	77.795	1.00	27.69		O
ANISOU	945	OG	SER	A	513	3642	3068	3810	241	217	-215	O
ATOM	946	N	HIS	A	514	17.661	36.294	77.584	1.00	19.42		N
ANISOU	946	N	HIS	A	514	2705	2009	2664	46	179	207	N
ATOM	947	CA	HIS	A	514	18.077	35.398	78.679	1.00	18.23		C
ANISOU	947	CA	HIS	A	514	2600	1942	2384	76	155	-16	C
ATOM	948	C	HIS	A	514	17.852	33.956	78.254	1.00	16.65		C
ANISOU	948	C	HIS	A	514	2091	1960	2275	3	97	-18	C
ATOM	949	O	HIS	A	514	17.070	33.726	77.331	1.00	18.87		O
ANISOU	949	O	HIS	A	514	2639	2068	2462	176	-225	164	O
ATOM	950	CB	HIS	A	514	17.171	35.673	79.900	1.00	18.92		C
ANISOU	950	CB	HIS	A	514	2673	2202	2315	6	188	112	C
ATOM	951	CG	HIS	A	514	17.591	34.942	81.132	1.00	19.11		C
ANISOU	951	CG	HIS	A	514	2472	2322	2468	89	136	70	C
ATOM	952	ND1	HIS	A	514	18.865	34.979	81.688	1.00	19.64		N
ANISOU	952	ND1	HIS	A	514	2736	2434	2293	169	110	164	N
ATOM	953	CD2	HIS	A	514	16.809	34.198	81.942	1.00	19.33		C
ANISOU	953	CD2	HIS	A	514	2766	2312	2266	190	221	-38	C
ATOM	954	CE1	HIS	A	514	18.834	34.229	82.799	1.00	20.67		C
ANISOU	954	CE1	HIS	A	514	2913	2558	2382	116	204	127	C
ATOM	955	NE2	HIS	A	514	17.611	33.760	82.956	1.00	18.73		N
ANISOU	955	NE2	HIS	A	514	2531	2269	2316	109	107	-78	N
ATOM	956	N	TRP	A	515	18.625	33.043	78.840	1.00	15.92		N
ANISOU	956	N	TRP	A	515	2444	1538	2069	-36	196	-66	N
ATOM	957	CA	TRP	A	515	18.452	31.617	78.550	1.00	15.22		C
ANISOU	957	CA	TRP	A	515	2159	1643	1980	-20	208	-57	C
ATOM	958	C	TRP	A	515	18.080	30.936	79.876	1.00	14.54		C
ANISOU	958	C	TRP	A	515	1759	1713	2052	33	265	-57	C
ATOM	959	O	TRP	A	515	18.694	31.235	80.873	1.00	15.86		O
ANISOU	959	O	TRP	A	515	2185	1588	2253	75	166	11	O
ATOM	960	CB	TRP	A	515	19.824	31.063	78.074	1.00	15.42		C
ANISOU	960	CB	TRP	A	515	2021	1862	1978	77	91	34	C
ATOM	961	CG	TRP	A	515	20.283	31.451	76.692	1.00	15.37		C
ANISOU	961	CG	TRP	A	515	1902	1948	1991	126	-47	153	C
ATOM	962	CD1	TRP	A	515	21.363	32.251	76.387	1.00	15.39		C
ANISOU	962	CD1	TRP	A	515	2241	1728	1878	61	-1	232	C
ATOM	963	CD2	TRP	A	515	19.731	31.037	75.433	1.00	14.53		C
ANISOU	963	CD2	TRP	A	515	1884	1593	2045	224	54	-11	C
ATOM	964	NE1	TRP	A	515	21.505	32.333	75.026	1.00	15.87		N
ANISOU	964	NE1	TRP	A	515	2067	2032	1932	-107	-121	94	N
ATOM	965	CE2	TRP	A	515	20.501	31.604	74.419	1.00	15.72		C
ANISOU	965	CE2	TRP	A	515	2216	1651	2106	64	-41	1	C
ATOM	966	CE3	TRP	A	515	18.659	30.194	75.094	1.00	16.46		C
ANISOU	966	CE3	TRP	A	515	2252	1816	2186	94	-211	-40	C
ATOM	967	CZ2	TRP	A	515	20.261	31.407	73.064	1.00	16.54		C
ANISOU	967	CZ2	TRP	A	515	2189	1984	2110	61	45	76	C
ATOM	968	CZ3	TRP	A	515	18.420	29.985	73.742	1.00	17.08		C
ANISOU	968	CZ3	TRP	A	515	2443	2024	2021	144	28	114	C
ATOM	969	CH2	TRP	A	515	19.202	30.604	72.747	1.00	16.82		C
ANISOU	969	CH2	TRP	A	515	2107	2095	2188	94	66	19	C
ATOM	970	N	ALA	A	516	17.177	29.933	79.790	1.00	15.66		N
ANISOU	970	N	ALA	A	516	2188	1663	2100	-43	248	88	N

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ATOM    971  CA  ALA A 516      16.818  29.128  80.964  1.00 15.16           C
ANISOU  971  CA  ALA A 516    1918   1825   2019    -47    221    -70       C
ATOM    972  C   ALA A 516      16.616  27.692  80.445  1.00 15.33           C
ANISOU  972  C   ALA A 516    1861   1857   2107   -135     87    -64       C
ATOM    973  O   ALA A 516      16.833  27.425  79.244  1.00 14.82           O
ANISOU  973  O   ALA A 516    1910   1704   2018    -83     53     67       O
ATOM    974  CB  ALA A 516      15.612  29.648  81.735  1.00 16.96           C
ANISOU  974  CB  ALA A 516    2327   1740   2378     30    354    -70       C
ATOM    975  N   LEU A 517      16.205  26.789  81.303  1.00 17.24           N
ANISOU  975  N   LEU A 517    2556   1839   2157    -63     38    -68       N
ATOM    976  CA  LEU A 517      16.102  25.382  80.859  1.00 16.67           C
ANISOU  976  CA  LEU A 517    2261   1740   2331   -205    115    -18       C
ATOM    977  C   LEU A 517      14.928  24.654  81.483  1.00 16.87           C
ANISOU  977  C   LEU A 517    2301   1702   2408   -126    214      2       C
ATOM    978  O   LEU A 517      14.633  24.806  82.660  1.00 17.92           O
ANISOU  978  O   LEU A 517    2620   1695   2493   -226     46    -47       O
ATOM    979  CB  LEU A 517      17.380  24.700  81.401  1.00 17.54           C
ANISOU  979  CB  LEU A 517    2187   1807   2670    -79    140    -39       C
ATOM    980  CG  LEU A 517      17.538  23.199  81.135  1.00 16.59           C
ANISOU  980  CG  LEU A 517    2074   1810   2420    -31     92    -35       C
ATOM    981  CD1 LEU A 517      17.695  22.984  79.632  1.00 18.96           C
ANISOU  981  CD1 LEU A 517    2741   2017   2445    104     33   -124       C
ATOM    982  CD2 LEU A 517      18.763  22.599  81.870  1.00 16.79           C
ANISOU  982  CD2 LEU A 517    2199   1852   2331     49     76    -57       C
ATOM    983  N   GLY A 518      14.300  23.846  80.615  1.00 16.34           N
ANISOU  983  N   GLY A 518    1852   1842   2514   -188     65     28       N
ATOM    984  CA  GLY A 518      13.259  22.949  81.118  1.00 17.73           C
ANISOU  984  CA  GLY A 518    2289   1935   2511   -197    278     12       C
ATOM    985  C   GLY A 518      13.857  21.543  81.157  1.00 18.49           C
ANISOU  985  C   GLY A 518    2443   2060   2523    -97    170     45       C
ATOM    986  O   GLY A 518      14.626  21.177  80.266  1.00 16.84           O
ANISOU  986  O   GLY A 518    2257   1525   2616   -236    156    -18       O
ATOM    987  N   ILE A 519      13.489  20.784  82.213  1.00 18.37           N
ANISOU  987  N   ILE A 519    2462   2085   2432    -64    312     28       N
ATOM    988  CA  ILE A 519      13.961  19.393  82.287  1.00 18.08           C
ANISOU  988  CA  ILE A 519    2190   2084   2596   -166     65    106       C
ATOM    989  C   ILE A 519      12.721  18.496  82.461  1.00 18.84           C
ANISOU  989  C   ILE A 519    2477   2050   2632   -218    178     68       C
ATOM    990  O   ILE A 519      12.097  18.576  83.513  1.00 18.98           O
ANISOU  990  O   ILE A 519    2520   2015   2675   -390    236    113       O
ATOM    991  CB  ILE A 519      14.928  19.165  83.434  1.00 18.19           C
ANISOU  991  CB  ILE A 519    2571   1902   2437    -31     65    277       C
ATOM    992  CG1 ILE A 519      16.160  20.087  83.379  1.00 18.07           C
ANISOU  992  CG1 ILE A 519    2194   2251   2421    -33    -20    117       C
ATOM    993  CG2 ILE A 519      15.457  17.705  83.457  1.00 18.79           C
ANISOU  993  CG2 ILE A 519    2457   1978   2706     89     32    147       C
ATOM    994  CD1 ILE A 519      17.203  19.991  84.485  1.00 19.76           C
ANISOU  994  CD1 ILE A 519    2621   2656   2233   -209     29    161       C
ATOM    995  N   ILE A 520      12.411  17.704  81.455  1.00 18.78           N
ANISOU  995  N   ILE A 520    2245   2275   2616   -395    131    158       N
ATOM    996  CA  ILE A 520      11.299  16.725  81.676  1.00 19.96           C
ANISOU  996  CA  ILE A 520    2445   2272   2866   -295    185     77       C
ATOM    997  C   ILE A 520      11.989  15.440  82.129  1.00 20.99           C
ANISOU  997  C   ILE A 520    2539   2467   2968   -177     92     40       C
ATOM    998  O   ILE A 520      12.770  14.877  81.375  1.00 20.55           O
ANISOU  998  O   ILE A 520    3031   1906   2869   -193    197    -63       O
ATOM    999  CB  ILE A 520      10.583  16.508  80.366  1.00 19.40           C
ANISOU  999  CB  ILE A 520    2298   2316   2757   -260    177     29       C
ATOM   1000  CG1 ILE A 520       9.862  17.790  79.936  1.00 21.11           C
ANISOU 1000  CG1 ILE A 520    2590   2625   2806     12     95     23       C
ATOM   1001  CG2 ILE A 520       9.585  15.324  80.398  1.00 20.96           C
ANISOU 1001  CG2 ILE A 520    2654   2379   2933   -392    102    -83       C
ATOM   1002  CD1 ILE A 520       9.506  17.824  78.463  1.00 22.20           C
ANISOU 1002  CD1 ILE A 520    2753   2912   2769    -36    130     99       C
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ATOM   1003  N   ASP A 521      11.704  14.978  83.334  1.00 23.09           N
ANISOU 1003  N   ASP A 521    3058   2744   2971   -180     38     13       N
ATOM   1004  CA  ASP A 521      12.301  13.744  83.832  1.00 23.20           C
ANISOU 1004  CA  ASP A 521    2777   2744   3294   -218     31     81       C
ATOM   1005  C   ASP A 521      11.200  12.666  83.801  1.00 23.64           C
ANISOU 1005  C   ASP A 521    3012   2765   3204   -287    -55     29       C
ATOM   1006  O   ASP A 521      10.411  12.644  84.734  1.00 22.75           O
ANISOU 1006  O   ASP A 521    2999   2369   3276   -408      8   -135       O
ATOM   1007  CB  ASP A 521      12.816  13.930  85.247  1.00 25.50           C
ANISOU 1007  CB  ASP A 521    3215   3212   3263   -161     60     42       C
ATOM   1008  CG  ASP A 521      13.805  12.842  85.638  1.00 27.77           C
ANISOU 1008  CG  ASP A 521    3326   3511   3714     48     28     96       C
ATOM   1009  OD1 ASP A 521      13.532  11.677  85.267  1.00 28.61           O
ANISOU 1009  OD1 ASP A 521    3384   3609   3878    -30    -11     78       O
ATOM   1010  OD2 ASP A 521      14.841  13.167  86.293  1.00 30.97           O
ANISOU 1010  OD2 ASP A 521    3687   4027   4054   -123    -37     30       O
ATOM   1011  N   LEU A 522      11.239  11.868  82.746  1.00 24.20           N
ANISOU 1011  N   LEU A 522    3116   2732   3348   -304    127     26       N
ATOM   1012  CA  LEU A 522      10.199  10.834  82.599  1.00 25.59           C
ANISOU 1012  CA  LEU A 522    3039   3104   3579   -334    -29     46       C
ATOM   1013  C   LEU A 522      10.306   9.771  83.657  1.00 27.15           C
ANISOU 1013  C   LEU A 522    3284   3354   3677    -85     58    163       C
ATOM   1014  O   LEU A 522       9.276   9.216  84.106  1.00 27.20           O
ANISOU 1014  O   LEU A 522    3334   3290   3711   -238    -74    258       O
ATOM   1015  CB  LEU A 522      10.309  10.306  81.137  1.00 26.24           C
ANISOU 1015  CB  LEU A 522    3236   3094   3640   -249     56    -64       C
ATOM   1016  CG  LEU A 522      10.044  11.460  80.162  1.00 29.23           C
ANISOU 1016  CG  LEU A 522    3716   3702   3687    105     -2     91       C
ATOM   1017  CD1 LEU A 522      10.999  11.499  78.980  1.00 28.63           C
ANISOU 1017  CD1 LEU A 522    3741   3414   3724     56     72    122       C
ATOM   1018  CD2 LEU A 522       8.578  11.590  79.786  1.00 28.59           C
ANISOU 1018  CD2 LEU A 522    3622   3424   3818   -180     26     35       C
ATOM   1019  N   LYS A 523      11.518   9.444  84.086  1.00 29.20           N
ANISOU 1019  N   LYS A 523    3423   3708   3964   -255    -71    154       N
ATOM   1020  CA  LYS A 523      11.695   8.410  85.115  1.00 31.44           C
ANISOU 1020  CA  LYS A 523    4022   3843   4080      6    -98    154       C
ATOM   1021  C   LYS A 523      11.222   8.884  86.469  1.00 30.80           C
ANISOU 1021  C   LYS A 523    3802   3719   4183      7     -3    128       C
ATOM   1022  O   LYS A 523      10.569   8.154  87.225  1.00 31.37           O
ANISOU 1022  O   LYS A 523    3915   3689   4314    -42    -65    297       O
ATOM   1023  CB  LYS A 523      13.175   8.019  85.128  1.00 34.12           C
ANISOU 1023  CB  LYS A 523    4074   4323   4568    -45     54      5       C
ATOM   1024  CG  LYS A 523      13.656   7.079  86.201  1.00 38.10           C
ANISOU 1024  CG  LYS A 523    4961   4694   4822     99    -15    141       C
ATOM   1025  CD  LYS A 523      15.127   7.308  86.553  1.00 41.94           C
ANISOU 1025  CD  LYS A 523    5187   5312   5435      1    -91     16       C
ATOM   1026  CE  LYS A 523      16.040   7.405  85.343  1.00 44.32           C
ANISOU 1026  CE  LYS A 523    5651   5660   5529     60     95     55       C
ATOM   1027  NZ  LYS A 523      17.378   7.975  85.628  1.00 46.06           N
ANISOU 1027  NZ  LYS A 523    5831   5913   5756    -60    -93     21       N
ATOM   1028  N   LYS A 524      11.497  10.140  86.836  1.00 29.18           N
ANISOU 1028  N   LYS A 524    3695   3597   3795    -13    -75    142       N
ATOM   1029  CA  LYS A 524      11.062  10.677  88.120  1.00 28.80           C
ANISOU 1029  CA  LYS A 524    3580   3516   3846     66    -20    123       C
ATOM   1030  C   LYS A 524       9.664  11.283  88.059  1.00 26.40           C
ANISOU 1030  C   LYS A 524    3340   3146   3544   -159     24     69       C
ATOM   1031  O   LYS A 524       9.092  11.648  89.103  1.00 27.09           O
ANISOU 1031  O   LYS A 524    3377   3269   3647    -24     35    106       O
ATOM   1032  CB  LYS A 524      12.032  11.744  88.654  1.00 29.66           C
ANISOU 1032  CB  LYS A 524    3768   3683   3818    -69     10     39       C
ATOM   1033  CG  LYS A 524      13.466  11.227  88.794  1.00 32.19           C
ANISOU 1033  CG  LYS A 524    3842   4190   4197     50    -12     56       C
ATOM   1034  CD  LYS A 524      14.444  12.342  89.164  1.00 34.05           C
ANISOU 1034  CD  LYS A 524    4289   4315   4334    -87      1    -29       C
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ATOM   1035  CE  LYS A 524      15.909  12.024  89.102  1.00 34.85           C
ANISOU 1035  CE  LYS A 524    4336   4517   4389    -39    -25    -51       C
ATOM   1036  NZ  LYS A 524      16.514  11.646  87.793  1.00 34.69           N
ANISOU 1036  NZ  LYS A 524    4213   4629   4338   -165     53     97       N
ATOM   1037  N   LYS A 525       9.092  11.343  86.867  1.00 24.54           N
ANISOU 1037  N   LYS A 525    3232   2630   3462   -213    127    220       N
ATOM   1038  CA  LYS A 525       7.767  11.927  86.682  1.00 25.62           C
ANISOU 1038  CA  LYS A 525    3131   3067   3538   -250    214    146       C
ATOM   1039  C   LYS A 525       7.744  13.356  87.188  1.00 26.16           C
ANISOU 1039  C   LYS A 525    3279   3153   3508   -149    284     59       C
ATOM   1040  O   LYS A 525       6.892  13.789  87.970  1.00 24.65           O
ANISOU 1040  O   LYS A 525    3034   2685   3646   -142    296     30       O
ATOM   1041  CB  LYS A 525       6.677  11.085  87.430  1.00 27.03           C
ANISOU 1041  CB  LYS A 525    3332   3291   3646   -308    276    240       C
ATOM   1042  CG  LYS A 525       6.569   9.777  86.665  1.00 29.09           C
ANISOU 1042  CG  LYS A 525    3763   3577   3712   -275    138     23       C
ATOM   1043  CD  LYS A 525       5.263   9.009  86.934  1.00 31.07           C
ANISOU 1043  CD  LYS A 525    3931   3731   4144   -391    169    102       C
ATOM   1044  CE  LYS A 525       5.340   7.779  86.019  1.00 32.76           C
ANISOU 1044  CE  LYS A 525    4224   3964   4260   -113    121    -40       C
ATOM   1045  NZ  LYS A 525       4.799   7.982  84.634  1.00 32.11           N
ANISOU 1045  NZ  LYS A 525    4195   3735   4271   -247    160    134       N
ATOM   1046  N   THR A 526       8.700  14.171  86.714  1.00 25.53           N
ANISOU 1046  N   THR A 526    3122   3163   3415   -168    239     97       N
ATOM   1047  CA  THR A 526       8.746  15.561  87.174  1.00 26.25           C
ANISOU 1047  CA  THR A 526    3440   3213   3320     -8    257     25       C
ATOM   1048  C   THR A 526       9.073  16.477  86.000  1.00 25.67           C
ANISOU 1048  C   THR A 526    3244   3074   3435   -154    227     28       C
ATOM   1049  O   THR A 526       9.617  15.957  85.041  1.00 24.31           O
ANISOU 1049  O   THR A 526    3257   2538   3443   -243    304    112       O
ATOM   1050  CB  THR A 526       9.789  15.899  88.241  1.00 27.95           C
ANISOU 1050  CB  THR A 526    3353   3631   3636      6    115     66       C
ATOM   1051  OG1 THR A 526      11.134  15.610  87.757  1.00 28.65           O
ANISOU 1051  OG1 THR A 526    3431   3840   3617    -23    231     38       O
ATOM   1052  CG2 THR A 526       9.626  15.163  89.556  1.00 29.00           C
ANISOU 1052  CG2 THR A 526    3572   3855   3591    -71    213     22       C
ATOM   1053  N   ILE A 527       8.557  17.689  86.045  1.00 26.15           N
ANISOU 1053  N   ILE A 527    3520   2973   3442   -183    293     93       N
ATOM   1054  CA  ILE A 527       8.913  18.681  85.013  1.00 25.72           C
ANISOU 1054  CA  ILE A 527    3438   3005   3331   -268    311    -10       C
ATOM   1055  C   ILE A 527       9.538  19.836  85.805  1.00 25.92           C
ANISOU 1055  C   ILE A 527    3337   2983   3528   -269    322    -38       C
ATOM   1056  O   ILE A 527       8.884  20.394  86.696  1.00 25.19           O
ANISOU 1056  O   ILE A 527    3346   2724   3502   -384    382     36       O
ATOM   1057  CB  ILE A 527       7.782  19.182  84.149  1.00 27.76           C
ANISOU 1057  CB  ILE A 527    3756   3288   3503   -198    185    118       C
ATOM   1058  CG1 ILE A 527       7.127  17.969  83.496  1.00 28.22           C
ANISOU 1058  CG1 ILE A 527    3810   3383   3529   -198     -1    116       C
ATOM   1059  CG2 ILE A 527       8.299  20.211  83.130  1.00 27.06           C
ANISOU 1059  CG2 ILE A 527    3894   3026   3359   -121    105     49       C
ATOM   1060  CD1 ILE A 527       5.896  18.128  82.355  1.00 28.80           C
ANISOU 1060  CD1 ILE A 527    3371   3693   3879   -214    -27    149       C
ATOM   1061  N   GLY A 528      10.773  20.197  85.417  1.00 23.68           N
ANISOU 1061  N   GLY A 528    3179   2589   3230   -100    322    -67       N
ATOM   1062  CA  GLY A 528      11.439  21.235  86.200  1.00 22.81           C
ANISOU 1062  CA  GLY A 528    3073   2565   3030   -163    179    105       C
ATOM   1063  C   GLY A 528      11.870  22.408  85.327  1.00 21.82           C
ANISOU 1063  C   GLY A 528    2935   2571   2784   -210    302     13       C
ATOM   1064  O   GLY A 528      12.145  22.227  84.130  1.00 21.67           O
ANISOU 1064  O   GLY A 528    3434   2090   2709   -316    324    118       O
ATOM   1065  N   TYR A 529      11.827  23.570  85.943  1.00 19.07           N
ANISOU 1065  N   TYR A 529    2557   2264   2423   -228    432    288       N
ATOM   1066  CA  TYR A 529      12.249  24.815  85.244  1.00 19.32           C
ANISOU 1066  CA  TYR A 529    2534   2140   2667    -71    173    302       C
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ATOM   1067  C   TYR A 529      13.436  25.315  86.040  1.00 20.01           C
ANISOU 1067  C   TYR A 529    2649   2308   2646    -15    174     67       C
ATOM   1068  O   TYR A 529      13.318  25.491  87.260  1.00 20.14           O
ANISOU 1068  O   TYR A 529    2515   2533   2604   -316    392    139       O
ATOM   1069  CB  TYR A 529      11.101  25.844  85.232  1.00 19.92           C
ANISOU 1069  CB  TYR A 529    2567   2258   2741    -13    180     66       C
ATOM   1070  CG  TYR A 529      11.593  27.177  84.663  1.00 19.55           C
ANISOU 1070  CG  TYR A 529    2497   2303   2629    -87    180     65       C
ATOM   1071  CD1 TYR A 529      11.836  27.317  83.300  1.00 19.22           C
ANISOU 1071  CD1 TYR A 529    2345   2387   2573   -129    118     52       C
ATOM   1072  CD2 TYR A 529      11.825  28.242  85.498  1.00 21.21           C
ANISOU 1072  CD2 TYR A 529    2756   2502   2800   -136    192     -9       C
ATOM   1073  CE1 TYR A 529      12.275  28.523  82.766  1.00 19.18           C
ANISOU 1073  CE1 TYR A 529    2320   2392   2573   -195     69    -36       C
ATOM   1074  CE2 TYR A 529      12.292  29.454  84.977  1.00 20.66           C
ANISOU 1074  CE2 TYR A 529    2508   2470   2873   -167    199     44       C
ATOM   1075  CZ  TYR A 529      12.478  29.588  83.629  1.00 19.62           C
ANISOU 1075  CZ  TYR A 529    2545   2147   2763   -154    133     -1       C
ATOM   1076  OH  TYR A 529      12.986  30.765  83.079  1.00 20.48           O
ANISOU 1076  OH  TYR A 529    2570   2316   2897   -321    401     29       O
ATOM   1077  N   VAL A 530      14.599  25.509  85.419  1.00 19.71           N
ANISOU 1077  N   VAL A 530    2583   2184   2721   -161    244    215       N
ATOM   1078  CA  VAL A 530      15.818  25.864  86.151  1.00 19.51           C
ANISOU 1078  CA  VAL A 530    2619   2202   2591    -49    261    158       C
ATOM   1079  C   VAL A 530      16.382  27.118  85.501  1.00 18.62           C
ANISOU 1079  C   VAL A 530    2445   2200   2429   -134    225     21       C
ATOM   1080  O   VAL A 530      16.599  27.123  84.306  1.00 19.34           O
ANISOU 1080  O   VAL A 530    2687   2294   2367   -271    166     61       O
ATOM   1081  CB  VAL A 530      16.807  24.679  86.249  1.00 21.91           C
ANISOU 1081  CB  VAL A 530    2857   2345   3124    -36    187     52       C
ATOM   1082  CG1 VAL A 530      17.413  24.267  84.933  1.00 24.00           C
ANISOU 1082  CG1 VAL A 530    3085   2880   3154     43    244     34       C
ATOM   1083  CG2 VAL A 530      17.857  24.947  87.297  1.00 22.89           C
ANISOU 1083  CG2 VAL A 530    2902   2691   3104    182     80      1       C
ATOM   1084  N   ASP A 531      16.541  28.148  86.313  1.00 18.01           N
ANISOU 1084  N   ASP A 531    2426   1966   2452   -183    389    124       N
ATOM   1085  CA  ASP A 531      16.922  29.466  85.757  1.00 17.65           C
ANISOU 1085  CA  ASP A 531    2484   1877   2344   -179    246     29       C
ATOM   1086  C   ASP A 531      18.005  30.005  86.684  1.00 17.93           C
ANISOU 1086  C   ASP A 531    2407   2089   2317   -161    142    112       C
ATOM   1087  O   ASP A 531      17.778  30.190  87.888  1.00 19.21           O
ANISOU 1087  O   ASP A 531    2771   2146   2384   -125    233    -33       O
ATOM   1088  CB  ASP A 531      15.637  30.285  85.686  1.00 18.96           C
ANISOU 1088  CB  ASP A 531    2561   2170   2472    -54     84     46       C
ATOM   1089  CG  ASP A 531      15.766  31.672  85.084  1.00 19.66           C
ANISOU 1089  CG  ASP A 531    2837   2185   2448     25     86     15       C
ATOM   1090  OD1 ASP A 531      16.844  32.274  85.205  1.00 20.25           O
ANISOU 1090  OD1 ASP A 531    2842   2265   2585      2    151     94       O
ATOM   1091  OD2 ASP A 531      14.731  32.150  84.536  1.00 19.95           O
ANISOU 1091  OD2 ASP A 531    2846   2166   2567    -31     43    240       O
ATOM   1092  N   SER A 532      19.120  30.473  86.080  1.00 17.40           N
ANISOU 1092  N   SER A 532    2264   1902   2446    -72    297    -76       N
ATOM   1093  CA  SER A 532      20.242  30.997  86.832  1.00 18.39           C
ANISOU 1093  CA  SER A 532    2611   2139   2239     65     64    -49       C
ATOM   1094  C   SER A 532      20.136  32.508  87.153  1.00 18.84           C
ANISOU 1094  C   SER A 532    2556   2203   2400   -177    156   -105       C
ATOM   1095  O   SER A 532      21.073  33.027  87.750  1.00 18.74           O
ANISOU 1095  O   SER A 532    2671   2009   2441   -196    152   -251       O
ATOM   1096  CB  SER A 532      21.592  30.748  86.133  1.00 17.93           C
ANISOU 1096  CB  SER A 532    2371   2432   2008    -23     14      97       C
ATOM   1097  OG  SER A 532      21.558  31.336  84.814  1.00 17.00           O
ANISOU 1097  OG  SER A 532    2459   2032   1970     45     31     69       O
ATOM   1098  N   LEU A 533      19.032  33.127  86.821  1.00 19.85           N
ANISOU 1098  N   LEU A 533    2745   2151   2645    -51    165   -141       N
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ATOM   1099  CA  LEU A 533      18.818  34.515  87.294  1.00 21.71           C
ANISOU 1099  CA  LEU A 533    3000   2246   3002    103    143   -166       C
ATOM   1100  C   LEU A 533      17.338  34.623  87.615  1.00 23.14           C
ANISOU 1100  C   LEU A 533    2965   2634   3193    -16     25   -200       C
ATOM   1101  O   LEU A 533      16.559  35.275  86.940  1.00 24.86           O
ANISOU 1101  O   LEU A 533    3149   3073   3224    203    -39   -264       O
ATOM   1102  CB  LEU A 533      19.395  35.556  86.329  1.00 24.34           C
ANISOU 1102  CB  LEU A 533    3307   2753   3186    -43    112     53       C
ATOM   1103  CG  LEU A 533      19.592  36.950  86.969  1.00 27.67           C
ANISOU 1103  CG  LEU A 533    3878   3059   3577     -9     -7   -174       C
ATOM   1104  CD1 LEU A 533      20.617  36.899  88.082  1.00 28.13           C
ANISOU 1104  CD1 LEU A 533    3716   3229   3745    -53    -34   -148       C
ATOM   1105  CD2 LEU A 533      20.033  37.930  85.892  1.00 29.92           C
ANISOU 1105  CD2 LEU A 533    3970   3511   3887   -111     88     17       C
ATOM   1106  N   SER A 534      16.952  33.948  88.691  1.00 25.11           N
ANISOU 1106  N   SER A 534    3066   3104   3372      7    133   -128       N
ATOM   1107  CA  SER A 534      15.539  33.920  89.094  1.00 29.12           C
ANISOU 1107  CA  SER A 534    3196   3881   3988    -80    190      9       C
ATOM   1108  C   SER A 534      15.349  34.300  90.550  1.00 33.77           C
ANISOU 1108  C   SER A 534    4280   4419   4134   -194     87   -119       C
ATOM   1109  O   SER A 534      16.094  33.806  91.401  1.00 34.44           O
ANISOU 1109  O   SER A 534    4366   4668   4052   -165    174    -72       O
ATOM   1110  CB  SER A 534      15.093  32.458  88.916  1.00 29.92           C
ANISOU 1110  CB  SER A 534    3380   3929   4061   -138    236   -206       C
ATOM   1111  OG  SER A 534      13.809  32.243  89.499  1.00 30.70           O
ANISOU 1111  OG  SER A 534    3575   3946   4142   -250    236   -478       O
ATOM   1112  N   ASN A 535      14.266  35.000  90.853  1.00 38.52           N
ANISOU 1112  N   ASN A 535    4635   4858   5144     -4     91    -59       N
ATOM   1113  CA  ASN A 535      13.945  35.281  92.263  1.00 42.88           C
ANISOU 1113  CA  ASN A 535    5476   5575   5240    -52    104    -85       C
ATOM   1114  C   ASN A 535      12.969  34.223  92.783  1.00 43.94           C
ANISOU 1114  C   ASN A 535    5602   5574   5519    -83     98    -69       C
ATOM   1115  O   ASN A 535      12.632  34.188  93.981  1.00 45.16           O
ANISOU 1115  O   ASN A 535    5794   5834   5529    -62    126    -57       O
ATOM   1116  CB  ASN A 535      13.426  36.693  92.496  1.00 45.09           C
ANISOU 1116  CB  ASN A 535    5725   5679   5729     67     19    -85       C
ATOM   1117  CG  ASN A 535      14.484  37.713  92.100  1.00 46.65           C
ANISOU 1117  CG  ASN A 535    5922   5870   5934    -51     50    -47       C
ATOM   1118  OD1 ASN A 535      15.647  37.604  92.509  1.00 47.97           O
ANISOU 1118  OD1 ASN A 535    6025   6115   6085     -9    -45    -24       O
ATOM   1119  ND2 ASN A 535      14.074  38.675  91.291  1.00 47.55           N
ANISOU 1119  ND2 ASN A 535    6070   5977   6019     -7    -34    -26       N
ATOM   1120  N   GLY A 536      12.547  33.322  91.888  1.00 43.16           N
ANISOU 1120  N   GLY A 536    5433   5605   5360    -84    167    -75       N
ATOM   1121  CA  GLY A 536      11.720  32.219  92.314  1.00 42.57           C
ANISOU 1121  CA  GLY A 536    5433   5440   5300    -46     75   -137       C
ATOM   1122  C   GLY A 536      10.448  32.026  91.523  1.00 41.44           C
ANISOU 1122  C   GLY A 536    5306   5268   5172     28    180   -107       C
ATOM   1123  O   GLY A 536      10.131  32.713  90.550  1.00 39.62           O
ANISOU 1123  O   GLY A 536    4959   4833   5261    114    206   -212       O
ATOM   1124  N   PRO A 537       9.723  30.984  91.954  1.00 41.72           N
ANISOU 1124  N   PRO A 537    5401   5191   5259    -40     70   -135       N
ATOM   1125  CA  PRO A 537       8.483  30.615  91.290  1.00 41.96           C
ANISOU 1125  CA  PRO A 537    5303   5353   5288     -2     71    -64       C
ATOM   1126  C   PRO A 537       7.735  31.886  90.963  1.00 42.20           C
ANISOU 1126  C   PRO A 537    5449   5319   5267    -37     26     13       C
ATOM   1127  O   PRO A 537       7.541  32.752  91.840  1.00 43.58           O
ANISOU 1127  O   PRO A 537    5645   5509   5405    -72     73   -119       O
ATOM   1128  CB  PRO A 537       7.775  29.709  92.267  1.00 41.74           C
ANISOU 1128  CB  PRO A 537    5338   5221   5301    -24     57    -95       C
ATOM   1129  CG  PRO A 537       8.837  29.154  93.161  1.00 42.31           C
ANISOU 1129  CG  PRO A 537    5387   5305   5385    -51     26    -60       C
ATOM   1130  CD  PRO A 537      10.021  30.077  93.079  1.00 41.98           C
ANISOU 1130  CD  PRO A 537    5279   5392   5279    -36     56    -94       C
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ATOM   1131  N   ASN A 538      7.373  32.010  89.698  1.00 40.61           N
ANISOU 1131  N   ASN A 538     5152   5124   5155   -133     72    -84       N
ATOM   1132  CA  ASN A 538      6.665  33.207  89.241  1.00 40.39           C
ANISOU 1132  CA  ASN A 538     5000   5184   5163    -68     83    -29       C
ATOM   1133  C   ASN A 538      5.666  32.746  88.191  1.00 40.25           C
ANISOU 1133  C   ASN A 538     5117   5067   5110    -62     90    -49       C
ATOM   1134  O   ASN A 538      5.601  31.531  87.935  1.00 38.37           O
ANISOU 1134  O   ASN A 538     4756   5040   4784    -16    181   -116       O
ATOM   1135  CB  ASN A 538      7.631  34.252  88.746  1.00 40.79           C
ANISOU 1135  CB  ASN A 538     5146   5171   5181   -104     40    -56       C
ATOM   1136  CG  ASN A 538      8.113  34.344  87.324  1.00 40.60           C
ANISOU 1136  CG  ASN A 538     4958   5219   5247   -122    124    -86       C
ATOM   1137  OD1 ASN A 538      7.702  33.768  86.304  1.00 39.52           O
ANISOU 1137  OD1 ASN A 538     4663   5054   5297   -206    276   -173       O
ATOM   1138  ND2 ASN A 538      9.072  35.272  87.179  1.00 39.93           N
ANISOU 1138  ND2 ASN A 538     4863   5104   5205    -82     84   -126       N
ATOM   1139  N   ALA A 539      4.879  33.635  87.608  1.00 40.78           N
ANISOU 1139  N   ALA A 539     5169   5078   5245     -3     85    -37       N
ATOM   1140  CA  ALA A 539      3.881  33.169  86.653  1.00 42.07           C
ANISOU 1140  CA  ALA A 539     5313   5294   5379    -94     30    -93       C
ATOM   1141  C   ALA A 539      4.394  32.797  85.284  1.00 41.87           C
ANISOU 1141  C   ALA A 539     5126   5298   5486   -154    184    -81       C
ATOM   1142  O   ALA A 539      3.795  31.916  84.631  1.00 42.02           O
ANISOU 1142  O   ALA A 539     4965   5298   5702   -109    146   -169       O
ATOM   1143  CB  ALA A 539      2.715  34.130  86.525  1.00 42.83           C
ANISOU 1143  CB  ALA A 539     5446   5328   5500    -33    -41    -28       C
ATOM   1144  N   MET A 540      5.467  33.394  84.771  1.00 39.76           N
ANISOU 1144  N   MET A 540     4991   4816   5300    -88     88   -104       N
ATOM   1145  CA  MET A 540      5.943  33.051  83.437  1.00 38.59           C
ANISOU 1145  CA  MET A 540     4789   4594   5278    -57     91    -65       C
ATOM   1146  C   MET A 540      6.507  31.619  83.445  1.00 34.13           C
ANISOU 1146  C   MET A 540     3847   4429   4691   -227    158     -6       C
ATOM   1147  O   MET A 540      6.464  30.884  82.468  1.00 33.31           O
ANISOU 1147  O   MET A 540     3620   4010   5025   -131    272    -88       O
ATOM   1148  CB  MET A 540      7.086  33.962  82.977  1.00 41.08           C
ANISOU 1148  CB  MET A 540     4953   5188   5467   -187    151     74       C
ATOM   1149  CG  MET A 540      7.068  35.406  83.355  1.00 43.85           C
ANISOU 1149  CG  MET A 540     5580   5375   5705     -6     20    -53       C
ATOM   1150  SD  MET A 540      5.603  36.403  83.157  1.00 46.11           S
ANISOU 1150  SD  MET A 540     5627   5748   6147    125    -70    -87       S
ATOM   1151  CE  MET A 540      4.761  35.658  81.751  1.00 46.44           C
ANISOU 1151  CE  MET A 540     5900   5811   5933     78    -64     33       C
ATOM   1152  N   SER A 541      7.070  31.282  84.564  1.00 31.86           N
ANISOU 1152  N   SER A 541     3746   3817   4544   -158    418     21       N
ATOM   1153  CA  SER A 541      7.710  29.986  84.853  1.00 31.27           C
ANISOU 1153  CA  SER A 541     3578   3869   4433   -112    282    -17       C
ATOM   1154  C   SER A 541      6.585  28.941  84.861  1.00 30.32           C
ANISOU 1154  C   SER A 541     3649   3616   4256    -71    225   -115       C
ATOM   1155  O   SER A 541      6.751  27.800  84.465  1.00 27.86           O
ANISOU 1155  O   SER A 541     2924   3616   4046    -18    555   -162       O
ATOM   1156  CB  SER A 541      8.515  30.046  86.103  1.00 33.71           C
ANISOU 1156  CB  SER A 541     4081   4255   4472   -199    121    -73       C
ATOM   1157  OG  SER A 541      8.029  29.890  87.404  1.00 35.03           O
ANISOU 1157  OG  SER A 541     4054   4791   4464   -143    144   -374       O
ATOM   1158  N   PHE A 542      5.397  29.413  85.315  1.00 28.90           N
ANISOU 1158  N   PHE A 542     3328   3510   4142    -72    146    -51       N
ATOM   1159  CA  PHE A 542      4.279  28.441  85.248  1.00 30.40           C
ANISOU 1159  CA  PHE A 542     3529   3766   4258   -158    163   -100       C
ATOM   1160  C   PHE A 542      3.792  28.145  83.865  1.00 28.18           C
ANISOU 1160  C   PHE A 542     3090   3480   4137    -38    262    -87       C
ATOM   1161  O   PHE A 542      3.495  26.954  83.605  1.00 28.28           O
ANISOU 1161  O   PHE A 542     2991   3444   4308    -17    294   -186       O
ATOM   1162  CB  PHE A 542      3.115  28.992  86.067  1.00 32.99           C
ANISOU 1162  CB  PHE A 542     3889   4161   4487    -22    290   -115       C
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ATOM   1163  CG  PHE A 542       3.352  28.591  87.485  1.00 35.58           C
ANISOU 1163  CG  PHE A 542    4335   4609   4575    -27     50     -3       C
ATOM   1164  CD1 PHE A 542       3.521  29.567  88.444  1.00 37.40           C
ANISOU 1164  CD1 PHE A 542    4758   4693   4760    -87     33    -70       C
ATOM   1165  CD2 PHE A 542       3.359  27.251  87.839  1.00 37.35           C
ANISOU 1165  CD2 PHE A 542    4793   4650   4749     22     48    -16       C
ATOM   1166  CE1 PHE A 542       3.724  29.213  89.767  1.00 38.62           C
ANISOU 1166  CE1 PHE A 542    4869   4968   4838     31     -6     49       C
ATOM   1167  CE2 PHE A 542       3.576  26.892  89.156  1.00 38.49           C
ANISOU 1167  CE2 PHE A 542    4888   4957   4780    -50     10     15       C
ATOM   1168  CZ  PHE A 542       3.739  27.878  90.110  1.00 38.82           C
ANISOU 1168  CZ  PHE A 542    4945   4898   4908    -47     12    -23       C
ATOM   1169  N   ALA A 543       3.679  29.131  82.988  1.00 27.61           N
ANISOU 1169  N   ALA A 543    3063   3463   3966    -24    176   -153       N
ATOM   1170  CA  ALA A 543       3.312  28.898  81.608  1.00 28.18           C
ANISOU 1170  CA  ALA A 543    3316   3458   3934     62    109    -32       C
ATOM   1171  C   ALA A 543       4.315  27.934  80.978  1.00 27.24           C
ANISOU 1171  C   ALA A 543    3100   3419   3832    -39    -43    -41       C
ATOM   1172  O   ALA A 543       3.891  27.090  80.197  1.00 27.41           O
ANISOU 1172  O   ALA A 543    3093   3300   4021    -91     43    -34       O
ATOM   1173  CB  ALA A 543       3.207  30.162  80.775  1.00 30.56           C
ANISOU 1173  CB  ALA A 543    3874   3596   4141     47     28     63       C
ATOM   1174  N   ILE A 544       5.619  28.080  81.245  1.00 24.40           N
ANISOU 1174  N   ILE A 544    2987   2720   3564   -110     26      0       N
ATOM   1175  CA  ILE A 544       6.597  27.158  80.714  1.00 23.25           C
ANISOU 1175  CA  ILE A 544    2809   2822   3203   -109    -13     83       C
ATOM   1176  C   ILE A 544       6.320  25.756  81.267  1.00 21.89           C
ANISOU 1176  C   ILE A 544    2410   2778   3129    -13     80     44       C
ATOM   1177  O   ILE A 544       6.329  24.846  80.452  1.00 22.55           O
ANISOU 1177  O   ILE A 544    2457   2733   3378   -308     59     30       O
ATOM   1178  CB  ILE A 544       8.035  27.606  81.064  1.00 23.69           C
ANISOU 1178  CB  ILE A 544    2751   2967   3281    -29     41     77       C
ATOM   1179  CG1 ILE A 544       8.336  28.899  80.280  1.00 24.17           C
ANISOU 1179  CG1 ILE A 544    2814   2955   3412   -190    -99     71       C
ATOM   1180  CG2 ILE A 544       9.080  26.559  80.732  1.00 23.76           C
ANISOU 1180  CG2 ILE A 544    2973   2883   3173      0    -53    -30       C
ATOM   1181  CD1 ILE A 544       9.606  29.597  80.759  1.00 24.04           C
ANISOU 1181  CD1 ILE A 544    2749   2965   3420   -194     53     92       C
ATOM   1182  N   LEU A 545       6.202  25.602  82.589  1.00 23.24           N
ANISOU 1182  N   LEU A 545    2815   2786   3229    -90     47    105       N
ATOM   1183  CA  LEU A 545       5.971  24.239  83.093  1.00 22.70           C
ANISOU 1183  CA  LEU A 545    2755   2763   3107     83    147     97       C
ATOM   1184  C   LEU A 545       4.719  23.633  82.517  1.00 23.03           C
ANISOU 1184  C   LEU A 545    2696   2820   3235     55    137     38       C
ATOM   1185  O   LEU A 545       4.740  22.456  82.099  1.00 22.91           O
ANISOU 1185  O   LEU A 545    2514   2725   3464    -50    277     67       O
ATOM   1186  CB  LEU A 545       5.975  24.256  84.626  1.00 23.22           C
ANISOU 1186  CB  LEU A 545    2832   2865   3127     17     -2    -49       C
ATOM   1187  CG  LEU A 545       7.316  24.654  85.247  1.00 23.44           C
ANISOU 1187  CG  LEU A 545    2968   2825   3114   -155     27    -19       C
ATOM   1188  CD1 LEU A 545       7.091  25.039  86.694  1.00 25.32           C
ANISOU 1188  CD1 LEU A 545    3398   3041   3181    -46     89     24       C
ATOM   1189  CD2 LEU A 545       8.294  23.497  85.144  1.00 23.99           C
ANISOU 1189  CD2 LEU A 545    3040   2933   3144   -124     71   -113       C
ATOM   1190  N   THR A 546       3.585  24.400  82.423  1.00 23.28           N
ANISOU 1190  N   THR A 546    2713   2810   3322     57    151    281       N
ATOM   1191  CA  THR A 546       2.410  23.752  81.835  1.00 23.36           C
ANISOU 1191  CA  THR A 546    2805   2868   3203    107    153    104       C
ATOM   1192  C   THR A 546       2.547  23.433  80.360  1.00 23.93           C
ANISOU 1192  C   THR A 546    2851   2892   3350    101    219     74       C
ATOM   1193  O   THR A 546       2.063  22.396  79.881  1.00 25.26           O
ANISOU 1193  O   THR A 546    2518   3265   3816    -11    308   -239       O
ATOM   1194  CB  THR A 546       1.134  24.602  82.122  1.00 23.80           C
ANISOU 1194  CB  THR A 546    2923   2874   3245    272    152    110       C
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ATOM   1195  OG1 THR A 546      1.275  25.892  81.529  1.00 25.40           O
ANISOU 1195  OG1 THR A 546     3111   3131   3409     81    287    289       O
ATOM   1196  CG2 THR A 546      1.013  24.808  83.628  1.00 25.03           C
ANISOU 1196  CG2 THR A 546     3109   3137   3263    163    215     23       C
ATOM   1197  N   ASP A 547      3.336  24.193  79.609  1.00 23.36           N
ANISOU 1197  N   ASP A 547     2731   2860   3284     12    188     24       N
ATOM   1198  CA  ASP A 547      3.586  23.924  78.212  1.00 22.59           C
ANISOU 1198  CA  ASP A 547     2640   2728   3216     17    159     71       C
ATOM   1199  C   ASP A 547      4.348  22.589  78.092  1.00 22.24           C
ANISOU 1199  C   ASP A 547     2607   2709   3134    -49    194     47       C
ATOM   1200  O   ASP A 547      3.981  21.843  77.203  1.00 23.03           O
ANISOU 1200  O   ASP A 547     2636   2636   3479   -243    321     67       O
ATOM   1201  CB  ASP A 547      4.468  25.026  77.571  1.00 24.02           C
ANISOU 1201  CB  ASP A 547     2977   2889   3261   -129     98     85       C
ATOM   1202  CG  ASP A 547      3.654  26.182  77.017  1.00 25.48           C
ANISOU 1202  CG  ASP A 547     2948   3175   3557     21     12    187       C
ATOM   1203  OD1 ASP A 547      2.412  26.058  77.030  1.00 27.64           O
ANISOU 1203  OD1 ASP A 547     3264   3496   3741   -106    -39    263       O
ATOM   1204  OD2 ASP A 547      4.222  27.221  76.576  1.00 24.33           O
ANISOU 1204  OD2 ASP A 547     2766   3161   3318    223    132    261       O
ATOM   1205  N   LEU A 548      5.324  22.377  78.963  1.00 22.87           N
ANISOU 1205  N   LEU A 548     2872   2491   3328    -61    256     47       N
ATOM   1206  CA  LEU A 548      6.120  21.147  78.866  1.00 21.74           C
ANISOU 1206  CA  LEU A 548     2446   2575   3240    -37    117    130       C
ATOM   1207  C   LEU A 548      5.230  19.963  79.288  1.00 22.05           C
ANISOU 1207  C   LEU A 548     2709   2620   3048   -161    154     51       C
ATOM   1208  O   LEU A 548      5.381  18.895  78.712  1.00 20.79           O
ANISOU 1208  O   LEU A 548     2505   2472   2922   -377    267    123       O
ATOM   1209  CB  LEU A 548      7.401  21.241  79.689  1.00 22.72           C
ANISOU 1209  CB  LEU A 548     2922   2632   3081    -84     26     68       C
ATOM   1210  CG  LEU A 548      8.365  22.349  79.186  1.00 23.16           C
ANISOU 1210  CG  LEU A 548     2879   2809   3111   -138     77    100       C
ATOM   1211  CD1 LEU A 548      9.459  22.500  80.226  1.00 23.26           C
ANISOU 1211  CD1 LEU A 548     2610   3008   3220   -185     57    106       C
ATOM   1212  CD2 LEU A 548      8.905  21.969  77.810  1.00 23.43           C
ANISOU 1212  CD2 LEU A 548     2988   2840   3076    -75     94    160       C
ATOM   1213  N   GLN A 549      4.357  20.172  80.279  1.00 22.85           N
ANISOU 1213  N   GLN A 549     2718   2776   3187   -245    176    -77       N
ATOM   1214  CA  GLN A 549      3.462  19.079  80.712  1.00 24.15           C
ANISOU 1214  CA  GLN A 549     2874   2976   3324   -284    269     74       C
ATOM   1215  C   GLN A 549      2.494  18.733  79.598  1.00 24.61           C
ANISOU 1215  C   GLN A 549     3038   3071   3241   -118    217     51       C
ATOM   1216  O   GLN A 549      2.283  17.554  79.279  1.00 24.12           O
ANISOU 1216  O   GLN A 549     2527   3132   3508   -389    233    175       O
ATOM   1217  CB  GLN A 549      2.712  19.459  82.007  1.00 25.04           C
ANISOU 1217  CB  GLN A 549     2996   3091   3425   -259    296    -52       C
ATOM   1218  CG  GLN A 549      1.749  18.311  82.410  1.00 26.70           C
ANISOU 1218  CG  GLN A 549     3371   3092   3684   -292    275     64       C
ATOM   1219  CD  GLN A 549      1.112  18.676  83.738  1.00 28.24           C
ANISOU 1219  CD  GLN A 549     3323   3531   3875    -84    361     61       C
ATOM   1220  OE1 GLN A 549      0.731  19.849  83.875  1.00 28.70           O
ANISOU 1220  OE1 GLN A 549     3378   3418   4109   -194    636     61       O
ATOM   1221  NE2 GLN A 549      1.067  17.723  84.652  1.00 28.03           N
ANISOU 1221  NE2 GLN A 549     3248   3564   3836   -151    289     70       N
ATOM   1222  N   LYS A 550      2.023  19.773  78.896  1.00 25.30           N
ANISOU 1222  N   LYS A 550     2979   3168   3468    -90    108    139       N
ATOM   1223  CA  LYS A 550      1.165  19.575  77.740  1.00 25.70           C
ANISOU 1223  CA  LYS A 550     3203   3128   3434   -228    126    145       C
ATOM   1224  C   LYS A 550      1.855  18.767  76.673  1.00 24.53           C
ANISOU 1224  C   LYS A 550     2856   3036   3429   -262     78    152       C
ATOM   1225  O   LYS A 550      1.333  17.855  76.045  1.00 23.16           O
ANISOU 1225  O   LYS A 550     2326   2988   3486   -472     81    361       O
ATOM   1226  CB  LYS A 550      0.712  20.937  77.181  1.00 28.22           C
ANISOU 1226  CB  LYS A 550     3592   3329   3799    -16    -29    166       C
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ATOM   1227  CG  LYS A 550      -0.155  20.713  75.941  1.00 31.76           C
ANISOU 1227  CG  LYS A 550     4057   4034   3977   -202   -152    -12       C
ATOM   1228  CD  LYS A 550      -0.798  22.002  75.495  1.00 34.48           C
ANISOU 1228  CD  LYS A 550     4395   4240   4465    -27    -84     67       C
ATOM   1229  CE  LYS A 550       0.218  23.051  75.036  1.00 36.00           C
ANISOU 1229  CE  LYS A 550     4448   4437   4793   -124    -73     91       C
ATOM   1230  NZ  LYS A 550      -0.506  24.249  74.503  1.00 36.21           N
ANISOU 1230  NZ  LYS A 550     4398   4531   4830   -109   -120    125       N
ATOM   1231  N   TYR A 551       3.145  19.062  76.396  1.00 22.08           N
ANISOU 1231  N   TYR A 551     2503   2664   3225   -274     86    195       N
ATOM   1232  CA  TYR A 551       3.909  18.345  75.403  1.00 20.84           C
ANISOU 1232  CA  TYR A 551     2400   2545   2972   -330   -107    215       C
ATOM   1233  C   TYR A 551       3.939  16.846  75.739  1.00 22.16           C
ANISOU 1233  C   TYR A 551     2678   2630   3111   -121    -82    136       C
ATOM   1234  O   TYR A 551       3.842  16.000  74.871  1.00 23.19           O
ANISOU 1234  O   TYR A 551     2812   2901   3100   -254   -184    114       O
ATOM   1235  CB  TYR A 551       5.375  18.882  75.293  1.00 19.68           C
ANISOU 1235  CB  TYR A 551     2346   2340   2791   -357    -31     87       C
ATOM   1236  CG  TYR A 551       6.163  18.079  74.261  1.00 19.76           C
ANISOU 1236  CG  TYR A 551     2121   2480   2908   -346     16    116       C
ATOM   1237  CD1 TYR A 551       5.966  18.245  72.892  1.00 19.83           C
ANISOU 1237  CD1 TYR A 551     2216   2489   2828   -431     36    -34       C
ATOM   1238  CD2 TYR A 551       7.059  17.110  74.685  1.00 20.99           C
ANISOU 1238  CD2 TYR A 551     2399   2410   3165   -388     45     41       C
ATOM   1239  CE1 TYR A 551       6.647  17.464  71.979  1.00 19.92           C
ANISOU 1239  CE1 TYR A 551     2278   2447   2845   -361    -42    -31       C
ATOM   1240  CE2 TYR A 551       7.770  16.333  73.799  1.00 19.81           C
ANISOU 1240  CE2 TYR A 551     2230   2390   2907   -358    -83    -65       C
ATOM   1241  CZ  TYR A 551       7.554  16.512  72.449  1.00 20.68           C
ANISOU 1241  CZ  TYR A 551     2485   2446   2925   -321    -18     79       C
ATOM   1242  OH  TYR A 551       8.268  15.769  71.555  1.00 21.83           O
ANISOU 1242  OH  TYR A 551     2357   2564   3373   -132   -156    -63       O
ATOM   1243  N   VAL A 552       4.265  16.533  76.986  1.00 21.72           N
ANISOU 1243  N   VAL A 552     2386   2787   3078   -120    -30    180       N
ATOM   1244  CA  VAL A 552       4.385  15.135  77.406  1.00 22.67           C
ANISOU 1244  CA  VAL A 552     2549   2802   3262   -149    -13    132       C
ATOM   1245  C   VAL A 552       3.043  14.392  77.218  1.00 23.51           C
ANISOU 1245  C   VAL A 552     2671   2936   3325   -258     -5     62       C
ATOM   1246  O   VAL A 552       3.042  13.279  76.656  1.00 24.33           O
ANISOU 1246  O   VAL A 552     2665   3018   3563   -221    -92     32       O
ATOM   1247  CB  VAL A 552       4.835  15.022  78.856  1.00 22.88           C
ANISOU 1247  CB  VAL A 552     2728   2733   3233   -267     -1    -12       C
ATOM   1248  CG1 VAL A 552       4.887  13.538  79.270  1.00 23.22           C
ANISOU 1248  CG1 VAL A 552     2805   2751   3266   -108    -86    143       C
ATOM   1249  CG2 VAL A 552       6.250  15.553  79.032  1.00 21.76           C
ANISOU 1249  CG2 VAL A 552     2469   2657   3142    -30   -118     65       C
ATOM   1250  N   MET A 553       1.989  15.073  77.663  1.00 23.62           N
ANISOU 1250  N   MET A 553     2690   2877   3407   -202    -72    195       N
ATOM   1251  CA  MET A 553       0.652  14.423  77.505  1.00 24.68           C
ANISOU 1251  CA  MET A 553     2803   2951   3624   -329    -27    129       C
ATOM   1252  C   MET A 553       0.296  14.201  76.061  1.00 26.17           C
ANISOU 1252  C   MET A 553     3177   3123   3644    -57    -15     61       C
ATOM   1253  O   MET A 553      -0.177  13.097  75.669  1.00 28.15           O
ANISOU 1253  O   MET A 553     3440   3305   3950   -389   -109     53       O
ATOM   1254  CB  MET A 553      -0.353  15.281  78.272  1.00 23.70           C
ANISOU 1254  CB  MET A 553     2706   2827   3473   -467     -1    177       C
ATOM   1255  CG  MET A 553      -0.220  15.213  79.787  1.00 26.39           C
ANISOU 1255  CG  MET A 553     3285   3188   3553   -376     45     88       C
ATOM   1256  SD  MET A 553      -1.312  16.315  80.696  1.00 29.71           S
ANISOU 1256  SD  MET A 553     3253   3855   4178   -231    342     92       S
ATOM   1257  CE  MET A 553      -1.514  17.756  79.686  1.00 31.97           C
ANISOU 1257  CE  MET A 553     3853   4196   4098   -122    147    142       C
ATOM   1258  N   GLU A 554       0.511  15.163  75.164  1.00 25.97           N
ANISOU 1258  N   GLU A 554     2964   3201   3703    -86      4    102       N
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ATOM   1259  CA  GLU A 554       0.181  15.005  73.757  1.00 27.16           C
ANISOU 1259  CA  GLU A 554    3313   3308   3698   -127    -18      1       C
ATOM   1260  C   GLU A 554       1.098  14.065  73.003  1.00 26.08           C
ANISOU 1260  C   GLU A 554    3038   3297   3576   -196   -102     47       C
ATOM   1261  O   GLU A 554       0.659  13.172  72.252  1.00 26.70           O
ANISOU 1261  O   GLU A 554    3074   3283   3790   -361   -293     12       O
ATOM   1262  CB  GLU A 554       0.117  16.374  73.050  1.00 29.34           C
ANISOU 1262  CB  GLU A 554    3799   3529   3820   -210    -66    159       C
ATOM   1263  CG  GLU A 554      -0.898  17.308  73.689  1.00 32.77           C
ANISOU 1263  CG  GLU A 554    4107   4049   4294     11     27    -15       C
ATOM   1264  CD  GLU A 554      -2.343  16.855  73.550  1.00 35.94           C
ANISOU 1264  CD  GLU A 554    4309   4585   4762   -137    -26      5       C
ATOM   1265  OE1 GLU A 554      -2.631  16.312  72.470  1.00 37.57           O
ANISOU 1265  OE1 GLU A 554    4520   4980   4775   -228   -112    -40       O
ATOM   1266  OE2 GLU A 554      -3.104  17.042  74.519  1.00 37.27           O
ANISOU 1266  OE2 GLU A 554    4434   4746   4980   -161     93     15       O
ATOM   1267  N   GLU A 555       2.411  14.166  73.183  1.00 24.96           N
ANISOU 1267  N   GLU A 555    2975   3048   3461   -271   -172     78       N
ATOM   1268  CA  GLU A 555       3.378  13.327  72.502  1.00 24.85           C
ANISOU 1268  CA  GLU A 555    2759   3221   3463   -315   -182    -14       C
ATOM   1269  C   GLU A 555       3.218  11.868  72.897  1.00 26.77           C
ANISOU 1269  C   GLU A 555    3176   3310   3686    -84   -143     59       C
ATOM   1270  O   GLU A 555       3.437  10.979  72.081  1.00 29.06           O
ANISOU 1270  O   GLU A 555    3680   3496   3868   -228    -53    -99       O
ATOM   1271  CB  GLU A 555       4.818  13.829  72.834  1.00 25.12           C
ANISOU 1271  CB  GLU A 555    2780   3207   3557   -214   -142   -116       C
ATOM   1272  CG  GLU A 555       5.884  13.047  72.095  1.00 24.32           C
ANISOU 1272  CG  GLU A 555    2804   3053   3384   -277   -116   -104       C
ATOM   1273  CD  GLU A 555       5.802  13.180  70.592  1.00 25.45           C
ANISOU 1273  CD  GLU A 555    3006   3215   3449   -194   -128    -23       C
ATOM   1274  OE1 GLU A 555       5.283  14.191  70.069  1.00 26.52           O
ANISOU 1274  OE1 GLU A 555    3194   3175   3709   -237   -137    -15       O
ATOM   1275  OE2 GLU A 555       6.302  12.257  69.917  1.00 25.01           O
ANISOU 1275  OE2 GLU A 555    2964   3115   3424   -181    -95     68       O
ATOM   1276  N   SER A 556       2.807  11.611  74.138  1.00 27.38           N
ANISOU 1276  N   SER A 556    3426   3272   3706   -160    -58     68       N
ATOM   1277  CA  SER A 556       2.605  10.236  74.590  1.00 28.32           C
ANISOU 1277  CA  SER A 556    3570   3307   3884   -260   -158     76       C
ATOM   1278  C   SER A 556       1.213   9.710  74.262  1.00 29.09           C
ANISOU 1278  C   SER A 556    3485   3512   4057   -240    -38     34       C
ATOM   1279  O   SER A 556       0.870   8.642  74.794  1.00 30.33           O
ANISOU 1279  O   SER A 556    3797   3389   4339   -335   -138      2       O
ATOM   1280  CB  SER A 556       2.796  10.137  76.107  1.00 27.22           C
ANISOU 1280  CB  SER A 556    3373   3170   3800   -195    -28     63       C
ATOM   1281  OG  SER A 556       1.787  10.829  76.803  1.00 26.02           O
ANISOU 1281  OG  SER A 556    2773   3122   3989   -399   -131    121       O
ATOM   1282  N   LYS A 557       0.404  10.484  73.579  1.00 30.03           N
ANISOU 1282  N   LYS A 557    3768   3536   4104   -271   -156     16       N
ATOM   1283  CA  LYS A 557      -0.977  10.070  73.286  1.00 32.80           C
ANISOU 1283  CA  LYS A 557    3756   4228   4479   -220    -63     41       C
ATOM   1284  C   LYS A 557      -1.721   9.825  74.577  1.00 33.23           C
ANISOU 1284  C   LYS A 557    3980   4202   4442   -136    -55     37       C
ATOM   1285  O   LYS A 557      -2.440   8.813  74.727  1.00 34.82           O
ANISOU 1285  O   LYS A 557    4210   4271   4749   -324   -139    -29       O
ATOM   1286  CB  LYS A 557      -0.924   8.833  72.392  1.00 34.77           C
ANISOU 1286  CB  LYS A 557    4195   4368   4648   -148   -102    -73       C
ATOM   1287  CG  LYS A 557      -0.517   9.177  70.965  1.00 38.01           C
ANISOU 1287  CG  LYS A 557    4704   4951   4787   -114     -3     33       C
ATOM   1288  CD  LYS A 557      -0.088   7.923  70.218  1.00 40.41           C
ANISOU 1288  CD  LYS A 557    5065   5095   5196     -3    -16    -90       C
ATOM   1289  CE  LYS A 557       0.416   8.299  68.825  1.00 42.43           C
ANISOU 1289  CE  LYS A 557    5443   5425   5252    -33     16      9       C
ATOM   1290  NZ  LYS A 557       1.635   7.512  68.466  1.00 44.10           N
ANISOU 1290  NZ  LYS A 557    5512   5671   5574     47     47    -22       N
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ATOM   1291  N   HIS A 558      -1.604  10.765  75.502  1.00 32.60           N
ANISOU 1291  N   HIS A 558    3743   4183   4463   -187    -75     16       N
ATOM   1292  CA  HIS A 558      -2.246  10.757  76.800  1.00 33.68           C
ANISOU 1292  CA  HIS A 558    4072   4242   4482    -99    -14     35       C
ATOM   1293  C   HIS A 558      -1.999   9.509  77.618  1.00 33.69           C
ANISOU 1293  C   HIS A 558    4004   4189   4607    -55      5     17       C
ATOM   1294  O   HIS A 558      -2.929   9.008  78.287  1.00 35.32           O
ANISOU 1294  O   HIS A 558    4271   4416   4731    -80    201    169       O
ATOM   1295  CB  HIS A 558      -3.767  11.022  76.623  1.00 35.06           C
ANISOU 1295  CB  HIS A 558    4096   4524   4702    -69    -45     36       C
ATOM   1296  CG  HIS A 558      -3.906  12.416  76.059  1.00 36.32           C
ANISOU 1296  CG  HIS A 558    4365   4626   4807     30    -17     71       C
ATOM   1297  ND1 HIS A 558      -4.002  12.646  74.705  1.00 37.84           N
ANISOU 1297  ND1 HIS A 558    4643   4878   4855     33    -26     46       N
ATOM   1298  CD2 HIS A 558      -3.882  13.615  76.676  1.00 36.40           C
ANISOU 1298  CD2 HIS A 558    4386   4659   4786    -21    -48      6       C
ATOM   1299  CE1 HIS A 558      -4.071  13.957  74.501  1.00 37.74           C
ANISOU 1299  CE1 HIS A 558    4664   4836   4839    -51     26      9       C
ATOM   1300  NE2 HIS A 558      -4.001  14.557  75.675  1.00 37.69           N
ANISOU 1300  NE2 HIS A 558    4664   4849   4806    -83     17     46       N
ATOM   1301  N   THR A 559      -0.775   8.998  77.602  1.00 31.31           N
ANISOU 1301  N   THR A 559    3768   3728   4399   -297    -91     22       N
ATOM   1302  CA  THR A 559      -0.446   7.850  78.422  1.00 31.64           C
ANISOU 1302  CA  THR A 559    3894   3908   4220   -309    -12    118       C
ATOM   1303  C   THR A 559       0.316   8.269  79.664  1.00 31.07           C
ANISOU 1303  C   THR A 559    3985   3721   4100   -247     39    160       C
ATOM   1304  O   THR A 559       0.378   7.551  80.671  1.00 31.04           O
ANISOU 1304  O   THR A 559    4015   3561   4218   -350     46    222       O
ATOM   1305  CB  THR A 559       0.341   6.761  77.702  1.00 32.73           C
ANISOU 1305  CB  THR A 559    4065   4057   4314   -146    -24     73       C
ATOM   1306  OG1 THR A 559       1.490   7.238  76.996  1.00 32.65           O
ANISOU 1306  OG1 THR A 559    4065   3911   4432   -285    -45     66       O
ATOM   1307  CG2 THR A 559      -0.505   6.013  76.659  1.00 32.81           C
ANISOU 1307  CG2 THR A 559    4071   4159   4235   -215    -79    135       C
ATOM   1308  N   ILE A 560       1.098   9.370  79.523  1.00 28.80           N
ANISOU 1308  N   ILE A 560    3655   3444   3845   -136    -90     99       N
ATOM   1309  CA  ILE A 560       1.937   9.804  80.635  1.00 28.76           C
ANISOU 1309  CA  ILE A 560    3735   3393   3797     -4    -42     47       C
ATOM   1310  C   ILE A 560       1.943  11.325  80.725  1.00 27.06           C
ANISOU 1310  C   ILE A 560    3319   3330   3632   -181    -12     97       C
ATOM   1311  O   ILE A 560       1.502  12.002  79.780  1.00 25.47           O
ANISOU 1311  O   ILE A 560    3138   3136   3404   -365   -109    -50       O
ATOM   1312  CB  ILE A 560       3.402   9.351  80.550  1.00 30.47           C
ANISOU 1312  CB  ILE A 560    3790   3772   4013     16     16     50       C
ATOM   1313  CG1 ILE A 560       4.066   9.737  79.235  1.00 30.69           C
ANISOU 1313  CG1 ILE A 560    3822   3865   3973     21     15     40       C
ATOM   1314  CG2 ILE A 560       3.567   7.868  80.869  1.00 30.96           C
ANISOU 1314  CG2 ILE A 560    3886   3731   4145    -19    -16    -20       C
ATOM   1315  CD1 ILE A 560       5.570   9.465  79.241  1.00 30.76           C
ANISOU 1315  CD1 ILE A 560    3679   3999   4009    -81    -71     48       C
ATOM   1316  N   GLY A 561       2.295  11.821  81.907  1.00 26.90           N
ANISOU 1316  N   GLY A 561    3362   3190   3669   -126    -48     83       N
ATOM   1317  CA  GLY A 561       2.398  13.268  82.091  1.00 26.89           C
ANISOU 1317  CA  GLY A 561    3295   3170   3751   -242    -57    141       C
ATOM   1318  C   GLY A 561       1.403  13.967  82.959  1.00 29.30           C
ANISOU 1318  C   GLY A 561    3630   3540   3963    -83     22     29       C
ATOM   1319  O   GLY A 561       1.754  14.916  83.667  1.00 28.44           O
ANISOU 1319  O   GLY A 561    3166   3646   3994   -347     60     87       O
ATOM   1320  N   GLU A 562       0.123  13.551  83.033  1.00 31.92           N
ANISOU 1320  N   GLU A 562    3812   3912   4403   -289     12     88       N
ATOM   1321  CA  GLU A 562      -0.894  14.265  83.803  1.00 33.43           C
ANISOU 1321  CA  GLU A 562    4179   4112   4413    -85     83     39       C
ATOM   1322  C   GLU A 562      -0.685  14.344  85.300  1.00 31.31           C
ANISOU 1322  C   GLU A 562    3697   3829   4369   -172     73    120       C
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ATOM   1323  O   GLU A 562      -1.151  15.281  85.988  1.00 30.72           O
ANISOU 1323  O   GLU A 562    3742   3700   4229   -265    131    229       O
ATOM   1324  CB  GLU A 562      -2.281  13.699  83.422  1.00 38.48           C
ANISOU 1324  CB  GLU A 562    4420   5013   5189   -158    -73    -61       C
ATOM   1325  CG  GLU A 562      -2.677  12.442  84.171  1.00 43.17           C
ANISOU 1325  CG  GLU A 562    5524   5245   5634    -35     53    163       C
ATOM   1326  CD  GLU A 562      -4.082  11.974  83.808  1.00 46.65           C
ANISOU 1326  CD  GLU A 562    5690   5941   6094    -89    -65     13       C
ATOM   1327  OE1 GLU A 562      -4.977  12.830  83.576  1.00 47.41           O
ANISOU 1327  OE1 GLU A 562    5810   5960   6244     15    -30    -13       O
ATOM   1328  OE2 GLU A 562      -4.284  10.735  83.751  1.00 49.19           O
ANISOU 1328  OE2 GLU A 562    6253   6001   6437    -48    -10     42       O
ATOM   1329  N   ASP A 563       0.084  13.431  85.890  1.00 28.74           N
ANISOU 1329  N   ASP A 563    3271   3553   4096   -421    112     69       N
ATOM   1330  CA  ASP A 563       0.382  13.368  87.291  1.00 29.52           C
ANISOU 1330  CA  ASP A 563    3462   3712   4041   -212    185     74       C
ATOM   1331  C   ASP A 563       1.820  13.792  87.605  1.00 28.85           C
ANISOU 1331  C   ASP A 563    3391   3756   3815    -92     68     66       C
ATOM   1332  O   ASP A 563       2.248  13.622  88.744  1.00 28.02           O
ANISOU 1332  O   ASP A 563    3147   3722   3775   -141    263    121       O
ATOM   1333  CB  ASP A 563       0.161  11.936  87.827  1.00 32.05           C
ANISOU 1333  CB  ASP A 563    4080   3863   4233   -219    158    177       C
ATOM   1334  CG  ASP A 563       1.014  10.881  87.188  1.00 33.86           C
ANISOU 1334  CG  ASP A 563    4361   4082   4421    -81    192     79       C
ATOM   1335  OD1 ASP A 563       1.761  11.179  86.221  1.00 33.79           O
ANISOU 1335  OD1 ASP A 563    4295   3981   4562   -259    185    232       O
ATOM   1336  OD2 ASP A 563       0.998   9.670  87.573  1.00 35.37           O
ANISOU 1336  OD2 ASP A 563    4698   4219   4524    -95    223    297       O
ATOM   1337  N   PHE A 564       2.504  14.388  86.608  1.00 28.32           N
ANISOU 1337  N   PHE A 564    3435   3509   3816   -134     30     16       N
ATOM   1338  CA  PHE A 564       3.869  14.845  86.925  1.00 26.63           C
ANISOU 1338  CA  PHE A 564    3161   3432   3526    -54    242    103       C
ATOM   1339  C   PHE A 564       3.870  16.034  87.880  1.00 27.46           C
ANISOU 1339  C   PHE A 564    3417   3352   3666   -121    181    107       C
ATOM   1340  O   PHE A 564       2.951  16.876  87.830  1.00 28.83           O
ANISOU 1340  O   PHE A 564    3359   3570   4023     21     67    168       O
ATOM   1341  CB  PHE A 564       4.619  15.226  85.635  1.00 25.30           C
ANISOU 1341  CB  PHE A 564    3155   3120   3337    -60    166     16       C
ATOM   1342  CG  PHE A 564       5.184  14.097  84.823  1.00 23.86           C
ANISOU 1342  CG  PHE A 564    2835   2962   3269    -76     81     31       C
ATOM   1343  CD1 PHE A 564       4.664  12.810  84.786  1.00 25.17           C
ANISOU 1343  CD1 PHE A 564    3212   2965   3386    -98     89     83       C
ATOM   1344  CD2 PHE A 564       6.279  14.362  83.997  1.00 24.60           C
ANISOU 1344  CD2 PHE A 564    3173   3039   3135   -100     89    206       C
ATOM   1345  CE1 PHE A 564       5.247  11.848  83.996  1.00 24.83           C
ANISOU 1345  CE1 PHE A 564    3137   3070   3228   -218     54      9       C
ATOM   1346  CE2 PHE A 564       6.862  13.391  83.236  1.00 25.49           C
ANISOU 1346  CE2 PHE A 564    3178   3121   3387   -210    130     21       C
ATOM   1347  CZ  PHE A 564       6.346  12.084  83.205  1.00 25.85           C
ANISOU 1347  CZ  PHE A 564    3282   3142   3396   -227     72     15       C
ATOM   1348  N   ASP A 565       4.894  16.155  88.717  1.00 27.01           N
ANISOU 1348  N   ASP A 565    3369   3467   3428   -112    231    327       N
ATOM   1349  CA  ASP A 565       5.046  17.272  89.628  1.00 30.49           C
ANISOU 1349  CA  ASP A 565    3846   3764   3974   -168    262     14       C
ATOM   1350  C   ASP A 565       5.778  18.401  88.872  1.00 30.83           C
ANISOU 1350  C   ASP A 565    3881   3829   4005    -90    262    104       C
ATOM   1351  O   ASP A 565       6.840  18.072  88.319  1.00 31.71           O
ANISOU 1351  O   ASP A 565    4021   3723   4302   -125    478      1       O
ATOM   1352  CB  ASP A 565       5.877  16.880  90.853  1.00 34.44           C
ANISOU 1352  CB  ASP A 565    4294   4408   4386    -13     15    135       C
ATOM   1353  CG  ASP A 565       5.699  17.779  92.064  1.00 37.62           C
ANISOU 1353  CG  ASP A 565    4837   4805   4652    -46     71    -62       C
ATOM   1354  OD1 ASP A 565       4.717  18.577  92.121  1.00 40.24           O
ANISOU 1354  OD1 ASP A 565    5238   4996   5054    143    156    -92       O
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ATOM   1355  OD2 ASP A 565       6.516  17.728  93.003  1.00 38.63           O
ANISOU 1355  OD2 ASP A 565    4933   4931   4814   -107      8     -1        O
ATOM   1356  N   LEU A 566       5.202  19.595  88.854  1.00 29.98           N
ANISOU 1356  N   LEU A 566    3876   3820   3693   -106    276     60        N
ATOM   1357  CA  LEU A 566       5.817  20.740  88.179  1.00 30.69           C
ANISOU 1357  CA  LEU A 566    3846   3857   3959   -155    273     54        C
ATOM   1358  C   LEU A 566       6.625  21.511  89.207  1.00 31.32           C
ANISOU 1358  C   LEU A 566    3889   3974   4039   -175    302    -41        C
ATOM   1359  O   LEU A 566       6.082  21.906  90.256  1.00 31.88           O
ANISOU 1359  O   LEU A 566    4061   3950   4101   -311    440   -145        O
ATOM   1360  CB  LEU A 566       4.771  21.619  87.510  1.00 32.50           C
ANISOU 1360  CB  LEU A 566    4165   4051   4133    -30    140     86        C
ATOM   1361  CG  LEU A 566       3.753  20.999  86.573  1.00 32.34           C
ANISOU 1361  CG  LEU A 566    4113   3941   4233    -74    147     37        C
ATOM   1362  CD1 LEU A 566       2.804  21.979  85.892  1.00 34.10           C
ANISOU 1362  CD1 LEU A 566    4423   4203   4330      2     96    117        C
ATOM   1363  CD2 LEU A 566       4.410  20.150  85.495  1.00 33.68           C
ANISOU 1363  CD2 LEU A 566    4321   4277   4201     -5    160    -15        C
ATOM   1364  N   ILE A 567       7.932  21.719  88.987  1.00 28.81           N
ANISOU 1364  N   ILE A 567    3728   3373   3848    -51    290     95        N
ATOM   1365  CA  ILE A 567       8.763  22.332  90.009  1.00 28.23           C
ANISOU 1365  CA  ILE A 567    3572   3500   3657    -99    358    153        C
ATOM   1366  C   ILE A 567       9.680  23.441  89.482  1.00 26.45           C
ANISOU 1366  C   ILE A 567    3392   3251   3409    -13    152    101        C
ATOM   1367  O   ILE A 567      10.130  23.274  88.350  1.00 25.65           O
ANISOU 1367  O   ILE A 567    3337   2913   3496     49    247    121        O
ATOM   1368  CB  ILE A 567       9.629  21.266  90.701  1.00 30.86           C
ANISOU 1368  CB  ILE A 567    3950   3828   3949    -20    158    286        C
ATOM   1369  CG1 ILE A 567      10.558  21.854  91.768  1.00 32.95           C
ANISOU 1369  CG1 ILE A 567    4180   4044   4296    -87    -11    174        C
ATOM   1370  CG2 ILE A 567      10.493  20.436  89.775  1.00 33.22           C
ANISOU 1370  CG2 ILE A 567    4314   4161   4146     40    183     98        C
ATOM   1371  CD1 ILE A 567       9.803  22.334  92.986  1.00 35.67           C
ANISOU 1371  CD1 ILE A 567    4647   4518   4388    -50     78     43        C
ATOM   1372  N   HIS A 568       9.807  24.516  90.224  1.00 24.84           N
ANISOU 1372  N   HIS A 568    3102   3302   3033    -61    145    208        N
ATOM   1373  CA  HIS A 568      10.759  25.581  89.879  1.00 25.70           C
ANISOU 1373  CA  HIS A 568    3155   3457   3152   -146     39    134        C
ATOM   1374  C   HIS A 568      12.034  25.130  90.629  1.00 26.73           C
ANISOU 1374  C   HIS A 568    3310   3625   3222     57     66    117        C
ATOM   1375  O   HIS A 568      12.050  25.213  91.863  1.00 27.81           O
ANISOU 1375  O   HIS A 568    3427   3972   3166    -24     -6    196        O
ATOM   1376  CB  HIS A 568      10.274  26.945  90.324  1.00 27.99           C
ANISOU 1376  CB  HIS A 568    3593   3575   3466    -43     52     27        C
ATOM   1377  CG  HIS A 568      11.100  28.126  89.865  1.00 31.14           C
ANISOU 1377  CG  HIS A 568    4036   3871   3925   -196     95     52        C
ATOM   1378  ND1 HIS A 568      10.560  29.082  89.037  1.00 31.70           N
ANISOU 1378  ND1 HIS A 568    4013   3873   4159     46    146     11        N
ATOM   1379  CD2 HIS A 568      12.379  28.514  90.071  1.00 33.15           C
ANISOU 1379  CD2 HIS A 568    4084   4198   4315   -162     39     39        C
ATOM   1380  CE1 HIS A 568      11.485  30.007  88.750  1.00 32.74           C
ANISOU 1380  CE1 HIS A 568    4265   3912   4262    -44     10    -53        C
ATOM   1381  NE2 HIS A 568      12.590  29.695  89.372  1.00 32.32           N
ANISOU 1381  NE2 HIS A 568    4113   3897   4272    -26     19   -126        N
ATOM   1382  N   LEU A 569      12.987  24.543  89.901  1.00 25.62           N
ANISOU 1382  N   LEU A 569    3271   3325   3140    -43    239     315        N
ATOM   1383  CA  LEU A 569      14.184  23.990  90.507  1.00 27.08           C
ANISOU 1383  CA  LEU A 569    3364   3567   3360     -6    133     217        C
ATOM   1384  C   LEU A 569      15.212  25.016  90.919  1.00 28.36           C
ANISOU 1384  C   LEU A 569    3513   3742   3521    -60     36     187        C
ATOM   1385  O   LEU A 569      15.493  25.954  90.149  1.00 29.04           O
ANISOU 1385  O   LEU A 569    3578   3840   3615   -195     68     312        O
ATOM   1386  CB  LEU A 569      14.881  23.040  89.496  1.00 28.77           C
ANISOU 1386  CB  LEU A 569    3662   3640   3628     70    193    103        C
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ATOM   1387  CG  LEU A 569      14.059  21.884  88.940  1.00 31.08           C
ANISOU 1387  CG  LEU A 569    3961   3909   3940    -25    110    -85       C
ATOM   1388  CD1 LEU A 569      14.730  21.287  87.700  1.00 30.23           C
ANISOU 1388  CD1 LEU A 569    3875   3692   3918    -64     86    -16       C
ATOM   1389  CD2 LEU A 569      13.837  20.810  90.005  1.00 32.36           C
ANISOU 1389  CD2 LEU A 569    4118   3988   4190    120     86     72       C
ATOM   1390  N   ASP A 570      15.805  24.873  92.082  1.00 28.26           N
ANISOU 1390  N   ASP A 570    3498   3877   3362      1    239    274       N
ATOM   1391  CA  ASP A 570      16.844  25.760  92.553  1.00 29.70           C
ANISOU 1391  CA  ASP A 570    3647   3905   3733    -38    194     88       C
ATOM   1392  C   ASP A 570      18.160  25.495  91.825  1.00 26.46           C
ANISOU 1392  C   ASP A 570    3306   3347   3401    -55    -19    182       C
ATOM   1393  O   ASP A 570      18.451  24.337  91.609  1.00 25.67           O
ANISOU 1393  O   ASP A 570    3032   3198   3522   -383    422    424       O
ATOM   1394  CB  ASP A 570      17.215  25.391  94.013  1.00 34.38           C
ANISOU 1394  CB  ASP A 570    4400   4612   4052      6    -90    179       C
ATOM   1395  CG  ASP A 570      16.044  25.734  94.911  1.00 37.90           C
ANISOU 1395  CG  ASP A 570    4636   5086   4680     44    129    -33       C
ATOM   1396  OD1 ASP A 570      15.544  26.859  94.700  1.00 40.78           O
ANISOU 1396  OD1 ASP A 570    5161   5227   5107    130     22     32       O
ATOM   1397  OD2 ASP A 570      15.736  24.842  95.727  1.00 39.89           O
ANISOU 1397  OD2 ASP A 570    4875   5415   4867     24    160    151       O
ATOM   1398  N   CYS A 571      18.994  26.481  91.568  1.00 25.36           N
ANISOU 1398  N   CYS A 571    3286   3138   3213     61     32    321       N
ATOM   1399  CA  CYS A 571      20.318  26.223  91.010  1.00 23.70           C
ANISOU 1399  CA  CYS A 571    3352   2818   2836     49     91     50       C
ATOM   1400  C   CYS A 571      21.241  27.380  91.342  1.00 23.46           C
ANISOU 1400  C   CYS A 571    3208   2812   2892     28    171    138       C
ATOM   1401  O   CYS A 571      20.748  28.429  91.748  1.00 23.13           O
ANISOU 1401  O   CYS A 571    3183   2724   2883    -24    310    220       O
ATOM   1402  CB  CYS A 571      20.278  25.968  89.475  1.00 22.21           C
ANISOU 1402  CB  CYS A 571    3231   2509   2699    171    148    210       C
ATOM   1403  SG  CYS A 571      20.045  27.501  88.538  1.00 21.88           S
ANISOU 1403  SG  CYS A 571    3662   2459   2192     96    372    113       S
ATOM   1404  N   PRO A 572      22.548  27.222  91.217  1.00 24.54           N
ANISOU 1404  N   PRO A 572    3200   2947   3176      7    178     40       N
ATOM   1405  CA  PRO A 572      23.518  28.285  91.440  1.00 24.11           C
ANISOU 1405  CA  PRO A 572    3218   2836   3106     56    174     81       C
ATOM   1406  C   PRO A 572      23.171  29.463  90.534  1.00 23.17           C
ANISOU 1406  C   PRO A 572    3137   2779   2886    -51    148     16       C
ATOM   1407  O   PRO A 572      22.841  29.259  89.382  1.00 22.63           O
ANISOU 1407  O   PRO A 572    3190   2682   2727   -133    307    149       O
ATOM   1408  CB  PRO A 572      24.876  27.683  91.122  1.00 25.09           C
ANISOU 1408  CB  PRO A 572    3137   3059   3335     79    110     88       C
ATOM   1409  CG  PRO A 572      24.643  26.190  91.232  1.00 26.29           C
ANISOU 1409  CG  PRO A 572    3405   3154   3429   -151     50     17       C
ATOM   1410  CD  PRO A 572      23.218  25.967  90.760  1.00 24.99           C
ANISOU 1410  CD  PRO A 572    3202   2978   3315     44    151     87       C
ATOM   1411  N   GLN A 573      23.191  30.663  91.113  1.00 21.01           N
ANISOU 1411  N   GLN A 573    3038   2644   2303    -81    295    134       N
ATOM   1412  CA  GLN A 573      22.731  31.830  90.337  1.00 21.31           C
ANISOU 1412  CA  GLN A 573    2952   2581   2562     25    191     48       C
ATOM   1413  C   GLN A 573      23.958  32.538  89.749  1.00 21.12           C
ANISOU 1413  C   GLN A 573    2861   2722   2442    -37    166     16       C
ATOM   1414  O   GLN A 573      25.010  32.581  90.392  1.00 22.44           O
ANISOU 1414  O   GLN A 573    3115   2770   2641   -192    111     93       O
ATOM   1415  CB  GLN A 573      22.020  32.789  91.312  1.00 21.04           C
ANISOU 1415  CB  GLN A 573    2833   2769   2391    -95    130   -104       C
ATOM   1416  CG  GLN A 573      20.721  32.169  91.876  1.00 21.77           C
ANISOU 1416  CG  GLN A 573    2805   2889   2578     26    239    -49       C
ATOM   1417  CD  GLN A 573      19.661  31.965  90.827  1.00 23.08           C
ANISOU 1417  CD  GLN A 573    3171   2986   2614    -15    180    -41       C
ATOM   1418  OE1 GLN A 573      19.046  32.951  90.356  1.00 23.03           O
ANISOU 1418  OE1 GLN A 573    3086   3003   2660    125    314    -10       O
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ATOM   1419  NE2 GLN A 573      19.416  30.727  90.379  1.00 22.52           N
ANISOU 1419  NE2 GLN A 573    3255   2844   2459     55    306     49        N
ATOM   1420  N   GLN A 574      23.812  33.038  88.526  1.00 20.37           N
ANISOU 1420  N   GLN A 574    2923   2289   2526   -162    125    126        N
ATOM   1421  CA  GLN A 574      24.967  33.723  87.887  1.00 21.00           C
ANISOU 1421  CA  GLN A 574    2788   2536   2655   -225     48    -26        C
ATOM   1422  C   GLN A 574      25.221  35.048  88.588  1.00 21.03           C
ANISOU 1422  C   GLN A 574    2803   2462   2728    -96    115    -40        C
ATOM   1423  O   GLN A 574      24.270  35.792  88.897  1.00 20.78           O
ANISOU 1423  O   GLN A 574    2756   2377   2764   -203     51   -265        O
ATOM   1424  CB  GLN A 574      24.584  33.888  86.406  1.00 21.23           C
ANISOU 1424  CB  GLN A 574    2863   2623   2581    -24    279    155        C
ATOM   1425  CG  GLN A 574      23.446  34.893  86.183  1.00 22.92           C
ANISOU 1425  CG  GLN A 574    3015   2804   2888    -35     38     62        C
ATOM   1426  CD  GLN A 574      22.949  34.783  84.758  1.00 23.64           C
ANISOU 1426  CD  GLN A 574    3062   3021   2900    -95     34     91        C
ATOM   1427  OE1 GLN A 574      22.371  33.774  84.366  1.00 23.51           O
ANISOU 1427  OE1 GLN A 574    3291   2898   2742    -59    107    119        O
ATOM   1428  NE2 GLN A 574      23.236  35.797  83.948  1.00 24.35           N
ANISOU 1428  NE2 GLN A 574    3349   2886   3017   -177    -65    102        N
ATOM   1429  N   PRO A 575      26.489  35.441  88.705  1.00 20.01           N
ANISOU 1429  N   PRO A 575    2714   2225   2664   -105     42    -50        N
ATOM   1430  CA  PRO A 575      26.856  36.702  89.356  1.00 21.59           C
ANISOU 1430  CA  PRO A 575    3074   2403   2727   -130    -50    -53        C
ATOM   1431  C   PRO A 575      27.025  37.844  88.371  1.00 22.37           C
ANISOU 1431  C   PRO A 575    3188   2633   2678   -219     69     11        C
ATOM   1432  O   PRO A 575      27.517  38.919  88.750  1.00 25.00           O
ANISOU 1432  O   PRO A 575    3881   2758   2858   -423    101    -59        O
ATOM   1433  CB  PRO A 575      28.211  36.325  89.960  1.00 21.25           C
ANISOU 1433  CB  PRO A 575    2817   2454   2802   -119     79   -128        C
ATOM   1434  CG  PRO A 575      28.847  35.492  88.873  1.00 20.60           C
ANISOU 1434  CG  PRO A 575    2747   2276   2804    -76     88    -36        C
ATOM   1435  CD  PRO A 575      27.686  34.608  88.385  1.00 21.45           C
ANISOU 1435  CD  PRO A 575    2591   2479   3080    -64    -82     69        C
ATOM   1436  N   ASN A 576      26.620  37.623  87.130  1.00 21.02           N
ANISOU 1436  N   ASN A 576    3061   2327   2598   -112     54     85        N
ATOM   1437  CA  ASN A 576      26.821  38.599  86.049  1.00 19.66           C
ANISOU 1437  CA  ASN A 576    2870   2133   2467   -138     -7    -31        C
ATOM   1438  C   ASN A 576      25.662  38.544  85.081  1.00 19.65           C
ANISOU 1438  C   ASN A 576    2863   2157   2445    106     84    -20        C
ATOM   1439  O   ASN A 576      24.758  37.713  85.260  1.00 20.86           O
ANISOU 1439  O   ASN A 576    2867   2310   2750   -104     72     -9        O
ATOM   1440  CB  ASN A 576      28.154  38.398  85.322  1.00 19.47           C
ANISOU 1440  CB  ASN A 576    2697   2189   2512    -95   -112    -51        C
ATOM   1441  CG  ASN A 576      28.245  36.983  84.730  1.00 20.85           C
ANISOU 1441  CG  ASN A 576    2773   2331   2817    -49   -169   -107        C
ATOM   1442  OD1 ASN A 576      27.374  36.665  83.914  1.00 19.46           O
ANISOU 1442  OD1 ASN A 576    3092   1840   2461    -30   -274    121        O
ATOM   1443  ND2 ASN A 576      29.208  36.159  85.131  1.00 21.52           N
ANISOU 1443  ND2 ASN A 576    2989   2195   2993   -122    -90     96        N
ATOM   1444  N   GLY A 577      25.706  39.455  84.077  1.00 18.58           N
ANISOU 1444  N   GLY A 577    2819   1935   2307    165     27   -114        N
ATOM   1445  CA  GLY A 577      24.568  39.415  83.156  1.00 19.56           C
ANISOU 1445  CA  GLY A 577    2721   2208   2502    302     -5   -106        C
ATOM   1446  C   GLY A 577      24.797  38.665  81.855  1.00 19.64           C
ANISOU 1446  C   GLY A 577    2836   2245   2383     48    138     15        C
ATOM   1447  O   GLY A 577      23.850  38.716  81.066  1.00 22.23           O
ANISOU 1447  O   GLY A 577    3087   2518   2841    255    -44     27        O
ATOM   1448  N   TYR A 578      25.878  37.922  81.682  1.00 16.92           N
ANISOU 1448  N   TYR A 578    2714   1577   2137    -76    165     21        N
ATOM   1449  CA  TYR A 578      26.145  37.336  80.362  1.00 16.24           C
ANISOU 1449  CA  TYR A 578    2585   1616   1969    -66     24     85        C
ATOM   1450  C   TYR A 578      26.284  35.807  80.384  1.00 16.73           C
ANISOU 1450  C   TYR A 578    2584   1605   2170     22     28    -38        C
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ATOM   1451  O   TYR A 578      26.277  35.191  79.311  1.00 17.44           O
ANISOU 1451  O   TYR A 578    2695   1778   2152   -307    -43    -34       O
ATOM   1452  CB  TYR A 578      27.464  37.881  79.819  1.00 18.05           C
ANISOU 1452  CB  TYR A 578    2417   1988   2454    -51     -9    200       C
ATOM   1453  CG  TYR A 578      28.616  37.965  80.797  1.00 17.53           C
ANISOU 1453  CG  TYR A 578    2369   2120   2173   -157    100     80       C
ATOM   1454  CD1 TYR A 578      29.377  36.836  81.036  1.00 17.77           C
ANISOU 1454  CD1 TYR A 578    2327   2085   2339   -193     92    220       C
ATOM   1455  CD2 TYR A 578      28.955  39.125  81.509  1.00 17.90           C
ANISOU 1455  CD2 TYR A 578    2503   2039   2258   -265     23    192       C
ATOM   1456  CE1 TYR A 578      30.460  36.820  81.913  1.00 18.18           C
ANISOU 1456  CE1 TYR A 578    2563   2145   2199   -269    -51    201       C
ATOM   1457  CE2 TYR A 578      30.000  39.140  82.409  1.00 18.63           C
ANISOU 1457  CE2 TYR A 578    2506   2192   2381   -171    -48    211       C
ATOM   1458  CZ  TYR A 578      30.767  38.002  82.588  1.00 19.75           C
ANISOU 1458  CZ  TYR A 578    2728   2199   2576    -85    -60     26       C
ATOM   1459  OH  TYR A 578      31.839  38.006  83.459  1.00 20.94           O
ANISOU 1459  OH  TYR A 578    3103   2377   2475   -225   -188    383       O
ATOM   1460  N   ASP A 579      26.364  35.218  81.553  1.00 16.24           N
ANISOU 1460  N   ASP A 579    2383   1562   2224    -32   -128    -93       N
ATOM   1461  CA  ASP A 579      26.597  33.756  81.601  1.00 15.40           C
ANISOU 1461  CA  ASP A 579    2375   1479   1997   -149   -153     31       C
ATOM   1462  C   ASP A 579      25.363  32.895  81.521  1.00 15.59           C
ANISOU 1462  C   ASP A 579    2026   1757   2142     -1     35      9       C
ATOM   1463  O   ASP A 579      25.522  31.662  81.674  1.00 16.28           O
ANISOU 1463  O   ASP A 579    2433   1646   2108    -37    199      9       O
ATOM   1464  CB  ASP A 579      27.393  33.402  82.866  1.00 16.76           C
ANISOU 1464  CB  ASP A 579    2320   1856   2192   -222   -213    171       C
ATOM   1465  CG  ASP A 579      28.892  33.467  82.657  1.00 18.53           C
ANISOU 1465  CG  ASP A 579    2559   2127   2355     55    -69     56       C
ATOM   1466  OD1 ASP A 579      29.395  33.366  81.509  1.00 18.83           O
ANISOU 1466  OD1 ASP A 579    2163   2493   2500    -31    -71    125       O
ATOM   1467  OD2 ASP A 579      29.610  33.626  83.673  1.00 20.44           O
ANISOU 1467  OD2 ASP A 579    2765   2218   2782     59   -321    171       O
ATOM   1468  N   CYS A 580      24.182  33.463  81.341  1.00 14.58           N
ANISOU 1468  N   CYS A 580    1786   1749   2004   -121    -45      4       N
ATOM   1469  CA  CYS A 580      22.970  32.593  81.394  1.00 14.75           C
ANISOU 1469  CA  CYS A 580    1887   1776   1941   -146     73     49       C
ATOM   1470  C   CYS A 580      23.109  31.389  80.475  1.00 15.30           C
ANISOU 1470  C   CYS A 580    2005   1882   1927   -119    -34     50       C
ATOM   1471  O   CYS A 580      22.645  30.293  80.890  1.00 15.92           O
ANISOU 1471  O   CYS A 580    2281   1646   2122    -91    156    -60       O
ATOM   1472  CB  CYS A 580      21.662  33.321  81.112  1.00 16.92           C
ANISOU 1472  CB  CYS A 580    2430   2088   1910    101     33     49       C
ATOM   1473  SG  CYS A 580      21.746  34.182  79.490  1.00 15.01           S
ANISOU 1473  SG  CYS A 580    2141   1455   2108     50    101     14       S
ATOM   1474  N   GLY A 581      23.559  31.538  79.246  1.00 15.26           N
ANISOU 1474  N   GLY A 581    2113   1666   2021     44    147    -83       N
ATOM   1475  CA  GLY A 581      23.611  30.365  78.313  1.00 15.15           C
ANISOU 1475  CA  GLY A 581    2305   1638   1815    -29   -224     -2       C
ATOM   1476  C   GLY A 581      24.626  29.341  78.879  1.00 12.80           C
ANISOU 1476  C   GLY A 581    1518   1669   1677   -133    135     98       C
ATOM   1477  O   GLY A 581      24.369  28.115  78.689  1.00 16.14           O
ANISOU 1477  O   GLY A 581    2411   1526   2194     74    128     65       O
ATOM   1478  N   ILE A 582      25.694  29.752  79.489  1.00 13.89           N
ANISOU 1478  N   ILE A 582    2309   1315   1655    145    100    105       N
ATOM   1479  CA  ILE A 582      26.664  28.816  80.097  1.00 11.67           C
ANISOU 1479  CA  ILE A 582     942   1769   1723      2     25    110       C
ATOM   1480  C   ILE A 582      25.980  28.097  81.274  1.00 14.76           C
ANISOU 1480  C   ILE A 582    2254   1734   1621    235    -19    111       C
ATOM   1481  O   ILE A 582      26.205  26.886  81.440  1.00 16.85           O
ANISOU 1481  O   ILE A 582    2551   1737   2117    -13     -5     89       O
ATOM   1482  CB  ILE A 582      27.966  29.614  80.495  1.00 14.03           C
ANISOU 1482  CB  ILE A 582    2097   1580   1655    -29   -270    186       C
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ATOM   1483  CG1 ILE A 582      28.659  29.974  79.220  1.00 15.12           C
ANISOU 1483  CG1 ILE A 582    1710   1814   2222     98    161    -32       C
ATOM   1484  CG2 ILE A 582      28.785  28.740  81.423  1.00 14.20           C
ANISOU 1484  CG2 ILE A 582    1517   1940   1938    -94   -207    270       C
ATOM   1485  CD1 ILE A 582      29.291  28.852  78.392  1.00 17.25           C
ANISOU 1485  CD1 ILE A 582    2564   2012   1976    -73    221   -182       C
ATOM   1486  N   TYR A 583      25.198  28.807  82.100  1.00 14.54           N
ANISOU 1486  N   TYR A 583    1670   1839   2016    -52    192     33       N
ATOM   1487  CA  TYR A 583      24.513  28.141  83.214  1.00 15.88           C
ANISOU 1487  CA  TYR A 583    2282   1866   1886     99     44     89       C
ATOM   1488  C   TYR A 583      23.505  27.151  82.647  1.00 14.88           C
ANISOU 1488  C   TYR A 583    1675   1970   2011    -51    -43     77       C
ATOM   1489  O   TYR A 583      23.331  26.047  83.234  1.00 16.28           O
ANISOU 1489  O   TYR A 583    2221   1849   2117     32    106      9       O
ATOM   1490  CB  TYR A 583      23.892  29.165  84.154  1.00 15.73           C
ANISOU 1490  CB  TYR A 583    2254   1807   1916      0    -54    -20       C
ATOM   1491  CG  TYR A 583      24.884  29.693  85.160  1.00 16.77           C
ANISOU 1491  CG  TYR A 583    1988   2161   2224    -35    -82     32       C
ATOM   1492  CD1 TYR A 583      25.956  30.477  84.772  1.00 16.09           C
ANISOU 1492  CD1 TYR A 583    2224   1720   2170     14     13    -41       C
ATOM   1493  CD2 TYR A 583      24.758  29.358  86.520  1.00 17.99           C
ANISOU 1493  CD2 TYR A 583    2333   2237   2264    -19     21     83       C
ATOM   1494  CE1 TYR A 583      26.870  30.952  85.725  1.00 16.44           C
ANISOU 1494  CE1 TYR A 583    2273   1814   2159      0   -103     65       C
ATOM   1495  CE2 TYR A 583      25.676  29.799  87.454  1.00 19.12           C
ANISOU 1495  CE2 TYR A 583    2700   2169   2395    -77     -3     48       C
ATOM   1496  CZ  TYR A 583      26.715  30.622  87.051  1.00 18.47           C
ANISOU 1496  CZ  TYR A 583    2359   2362   2296    -46     19     34       C
ATOM   1497  OH  TYR A 583      27.676  31.089  87.931  1.00 19.08           O
ANISOU 1497  OH  TYR A 583    2802   2068   2378    -85    -99    -10       O
ATOM   1498  N   VAL A 584      22.856  27.430  81.524  1.00 14.35           N
ANISOU 1498  N   VAL A 584    2297   1448   1706     -6     40     26       N
ATOM   1499  CA  VAL A 584      21.917  26.471  80.896  1.00 13.49           C
ANISOU 1499  CA  VAL A 584    1239   1687   2199    -25   -198    -53       C
ATOM   1500  C   VAL A 584      22.739  25.200  80.575  1.00 15.85           C
ANISOU 1500  C   VAL A 584    2076   1654   2293    -75     84   -156       C
ATOM   1501  O   VAL A 584      22.297  24.067  80.838  1.00 16.30           O
ANISOU 1501  O   VAL A 584    2203   1711   2280     38     89    137       O
ATOM   1502  CB  VAL A 584      21.225  27.070  79.676  1.00 14.64           C
ANISOU 1502  CB  VAL A 584    2065   1802   1698    148     93   -168       C
ATOM   1503  CG1 VAL A 584      20.504  25.998  78.788  1.00 16.28           C
ANISOU 1503  CG1 VAL A 584    2014   1854   2317   -183   -253   -128       C
ATOM   1504  CG2 VAL A 584      20.116  28.036  80.136  1.00 13.73           C
ANISOU 1504  CG2 VAL A 584    1648   1723   1846    126     74     24       C
ATOM   1505  N   CYS A 585      23.890  25.410  79.928  1.00 14.55           N
ANISOU 1505  N   CYS A 585    1829   1839   1861    149     84   -212       N
ATOM   1506  CA  CYS A 585      24.745  24.225  79.586  1.00 14.62           C
ANISOU 1506  CA  CYS A 585    1925   1546   2085     63     68   -103       C
ATOM   1507  C   CYS A 585      25.196  23.483  80.821  1.00 15.99           C
ANISOU 1507  C   CYS A 585    2138   1672   2266    166     93     24       C
ATOM   1508  O   CYS A 585      25.133  22.222  80.860  1.00 15.86           O
ANISOU 1508  O   CYS A 585    2047   1605   2374   -109    216   -105       O
ATOM   1509  CB  CYS A 585      25.953  24.692  78.743  1.00 16.25           C
ANISOU 1509  CB  CYS A 585    2385   1769   2019   -125    137    117       C
ATOM   1510  SG  CYS A 585      25.410  25.282  77.100  1.00 15.94           S
ANISOU 1510  SG  CYS A 585    2463   1609   1983    -35    232    134       S
ATOM   1511  N   MET A 586      25.607  24.149  81.898  1.00 16.65           N
ANISOU 1511  N   MET A 586    2185   1896   2246    -11     -3     75       N
ATOM   1512  CA  MET A 586      26.014  23.444  83.132  1.00 16.64           C
ANISOU 1512  CA  MET A 586    2076   1907   2338     20    -31    109       C
ATOM   1513  C   MET A 586      24.812  22.720  83.714  1.00 16.83           C
ANISOU 1513  C   MET A 586    2199   1798   2397     59     87     79       C
ATOM   1514  O   MET A 586      24.916  21.580  84.199  1.00 16.82           O
ANISOU 1514  O   MET A 586    2377   1660   2353     80    111     80       O
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ATOM   1515  CB  MET A 586      26.665  24.349  84.176  1.00 17.32           C
ANISOU 1515  CB  MET A 586    2143   2171   2266    -74    -39     84       C
ATOM   1516  CG  MET A 586      27.984  24.955  83.586  1.00 17.11           C
ANISOU 1516  CG  MET A 586    2322   2028   2150   -153    160    -64       C
ATOM   1517  SD  MET A 586      28.929  25.753  84.903  1.00 17.40           S
ANISOU 1517  SD  MET A 586    2281   1987   2344   -108    -37     71       S
ATOM   1518  CE  MET A 586      27.885  27.197  85.107  1.00 18.54           C
ANISOU 1518  CE  MET A 586    2749   1903   2393     33    -59    113       C
ATOM   1519  N   ASN A 587      23.624  23.345  83.747  1.00 14.87           N
ANISOU 1519  N   ASN A 587    1994   1530   2125    -56     81    -73       N
ATOM   1520  CA  ASN A 587      22.424  22.671  84.251  1.00 16.26           C
ANISOU 1520  CA  ASN A 587    1976   1864   2337     61    169     49       C
ATOM   1521  C   ASN A 587      22.050  21.459  83.429  1.00 16.93           C
ANISOU 1521  C   ASN A 587    2086   1969   2380    -52    -21     53       C
ATOM   1522  O   ASN A 587      21.545  20.458  84.021  1.00 19.17           O
ANISOU 1522  O   ASN A 587    2601   1963   2720    -43    137    198       O
ATOM   1523  CB  ASN A 587      21.243  23.661  84.322  1.00 16.58           C
ANISOU 1523  CB  ASN A 587    2216   1901   2184    196     62     55       C
ATOM   1524  CG  ASN A 587      21.249  24.420  85.628  1.00 17.93           C
ANISOU 1524  CG  ASN A 587    2440   2145   2227    135     83     81       C
ATOM   1525  OD1 ASN A 587      21.423  23.843  86.692  1.00 18.16           O
ANISOU 1525  OD1 ASN A 587    2542   2048   2309    197    181    210       O
ATOM   1526  ND2 ASN A 587      20.952  25.724  85.554  1.00 17.76           N
ANISOU 1526  ND2 ASN A 587    2369   2019   2361    122    345      2       N
ATOM   1527  N   THR A 588      22.316  21.472  82.133  1.00 17.13           N
ANISOU 1527  N   THR A 588    2480   1643   2386      9     28      9       N
ATOM   1528  CA  THR A 588      22.011  20.287  81.285  1.00 16.51           C
ANISOU 1528  CA  THR A 588    2153   1685   2436    -35     35     30       C
ATOM   1529  C   THR A 588      23.054  19.219  81.598  1.00 17.11           C
ANISOU 1529  C   THR A 588    2223   1914   2365     -6   -188     54       C
ATOM   1530  O   THR A 588      22.697  18.035  81.711  1.00 18.81           O
ANISOU 1530  O   THR A 588    2513   1878   2755   -142     75     40       O
ATOM   1531  CB  THR A 588      22.026  20.673  79.818  1.00 17.47           C
ANISOU 1531  CB  THR A 588    2187   2155   2297    172     -2   -123       C
ATOM   1532  OG1 THR A 588      21.090  21.795  79.642  1.00 16.25           O
ANISOU 1532  OG1 THR A 588    2279   1995   1900    185     19    146       O
ATOM   1533  CG2 THR A 588      21.626  19.570  78.851  1.00 18.62           C
ANISOU 1533  CG2 THR A 588    2485   2105   2483    206    -10   -123       C
ATOM   1534  N   LEU A 589      24.324  19.627  81.659  1.00 17.02           N
ANISOU 1534  N   LEU A 589    2103   1940   2424    138     30     66       N
ATOM   1535  CA  LEU A 589      25.396  18.656  81.965  1.00 16.26           C
ANISOU 1535  CA  LEU A 589    2115   1733   2330     29    -46     29       C
ATOM   1536  C   LEU A 589      25.164  17.998  83.308  1.00 17.93           C
ANISOU 1536  C   LEU A 589    2438   2010   2363     16    -91     52       C
ATOM   1537  O   LEU A 589      25.126  16.737  83.381  1.00 19.00           O
ANISOU 1537  O   LEU A 589    2729   1916   2573     93    -51     47       O
ATOM   1538  CB  LEU A 589      26.732  19.403  81.963  1.00 17.41           C
ANISOU 1538  CB  LEU A 589    2107   2050   2457     36    -46      3       C
ATOM   1539  CG  LEU A 589      27.962  18.670  82.523  1.00 17.90           C
ANISOU 1539  CG  LEU A 589    2019   2230   2553    108     64    -41       C
ATOM   1540  CD1 LEU A 589      28.251  17.540  81.558  1.00 20.93           C
ANISOU 1540  CD1 LEU A 589    2940   2349   2665     92    -74   -147       C
ATOM   1541  CD2 LEU A 589      29.115  19.669  82.572  1.00 19.00           C
ANISOU 1541  CD2 LEU A 589    2119   2499   2600    -83     24      4       C
ATOM   1542  N   TYR A 590      24.943  18.746  84.356  1.00 17.57           N
ANISOU 1542  N   TYR A 590    2164   2120   2393     -8    -66     -6       N
ATOM   1543  CA  TYR A 590      24.757  18.186  85.696  1.00 19.35           C
ANISOU 1543  CA  TYR A 590    2457   2321   2573   -163     88     69       C
ATOM   1544  C   TYR A 590      23.427  17.447  85.756  1.00 19.84           C
ANISOU 1544  C   TYR A 590    2584   2248   2707    -36    -78     68       C
ATOM   1545  O   TYR A 590      23.429  16.355  86.324  1.00 19.99           O
ANISOU 1545  O   TYR A 590    2457   2270   2868     76    -19    254       O
ATOM   1546  CB  TYR A 590      24.808  19.275  86.791  1.00 18.47           C
ANISOU 1546  CB  TYR A 590    2249   2297   2472    -75     74     29       C
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ATOM   1547  CG  TYR A 590      26.243  19.696  87.110  1.00 19.70           C
ANISOU 1547  CG  TYR A 590    2405   2494   2588   -166      9     41       C
ATOM   1548  CD1 TYR A 590      27.110  20.315  86.197  1.00 18.32           C
ANISOU 1548  CD1 TYR A 590    2317   2126   2519    -22   -137    177       C
ATOM   1549  CD2 TYR A 590      26.736  19.417  88.377  1.00 20.50           C
ANISOU 1549  CD2 TYR A 590    2611   2448   2730   -165   -113    179       C
ATOM   1550  CE1 TYR A 590      28.396  20.662  86.579  1.00 20.91           C
ANISOU 1550  CE1 TYR A 590    2746   2379   2820      3   -108    197       C
ATOM   1551  CE2 TYR A 590      28.015  19.757  88.767  1.00 22.19           C
ANISOU 1551  CE2 TYR A 590    2759   2738   2932   -119   -154    162       C
ATOM   1552  CZ  TYR A 590      28.845  20.365  87.839  1.00 21.25           C
ANISOU 1552  CZ  TYR A 590    2464   2849   2759   -119   -129     18       C
ATOM   1553  OH  TYR A 590      30.151  20.716  88.161  1.00 24.98           O
ANISOU 1553  OH  TYR A 590    2980   3270   3242   -111   -299     61       O
ATOM   1554  N   GLY A 591      22.369  18.004  85.199  1.00 17.96           N
ANISOU 1554  N   GLY A 591    2267   2041   2515    -97   -167     82       N
ATOM   1555  CA  GLY A 591      21.056  17.274  85.231  1.00 19.00           C
ANISOU 1555  CA  GLY A 591    2291   2242   2685    -41    -13    149       C
ATOM   1556  C   GLY A 591      21.187  15.972  84.452  1.00 20.19           C
ANISOU 1556  C   GLY A 591    2656   2328   2687   -117    -83    125       C
ATOM   1557  O   GLY A 591      20.603  14.978  84.956  1.00 21.39           O
ANISOU 1557  O   GLY A 591    2711   2305   3112    -15   -123    404       O
ATOM   1558  N   SER A 592      21.855  15.896  83.318  1.00 19.55           N
ANISOU 1558  N   SER A 592    2498   2220   2710   -110    -63     22       N
ATOM   1559  CA  SER A 592      21.994  14.639  82.554  1.00 20.81           C
ANISOU 1559  CA  SER A 592    2759   2333   2817     13    -20      9       C
ATOM   1560  C   SER A 592      22.749  13.574  83.332  1.00 22.20           C
ANISOU 1560  C   SER A 592    2799   2535   3102     47   -126     53       C
ATOM   1561  O   SER A 592      22.510  12.368  83.101  1.00 25.13           O
ANISOU 1561  O   SER A 592    3323   2530   3696    -15   -149    128       O
ATOM   1562  CB  SER A 592      22.702  14.845  81.216  1.00 21.67           C
ANISOU 1562  CB  SER A 592    2931   2516   2785     90    -47     78       C
ATOM   1563  OG  SER A 592      24.093  15.104  81.330  1.00 24.49           O
ANISOU 1563  OG  SER A 592    3197   2506   3603    -64    145     55       O
ATOM   1564  N   ALA A 593      23.678  14.020  84.183  1.00 21.83           N
ANISOU 1564  N   ALA A 593    2899   2455   2939     53   -171    177       N
ATOM   1565  CA  ALA A 593      24.477  13.086  84.997  1.00 21.91           C
ANISOU 1565  CA  ALA A 593    2652   2553   3121     35   -194    125       C
ATOM   1566  C   ALA A 593      23.834  12.838  86.339  1.00 22.32           C
ANISOU 1566  C   ALA A 593    2870   2523   3088   -153   -238    194       C
ATOM   1567  O   ALA A 593      24.409  12.103  87.194  1.00 23.63           O
ANISOU 1567  O   ALA A 593    3059   2628   3291    -63   -283    353       O
ATOM   1568  CB  ALA A 593      25.857  13.747  85.245  1.00 21.21           C
ANISOU 1568  CB  ALA A 593    2674   2296   3088    -20   -107     20       C
ATOM   1569  N   ASP A 594      22.661  13.384  86.612  1.00 23.59           N
ANISOU 1569  N   ASP A 594    3148   2496   3320    -37    -72    219       N
ATOM   1570  CA  ASP A 594      21.996  13.318  87.887  1.00 24.82           C
ANISOU 1570  CA  ASP A 594    3161   2833   3436   -159      2    159       C
ATOM   1571  C   ASP A 594      22.938  13.707  89.016  1.00 25.08           C
ANISOU 1571  C   ASP A 594    3164   2864   3500   -182    -92    281       C
ATOM   1572  O   ASP A 594      23.014  13.104  90.075  1.00 26.59           O
ANISOU 1572  O   ASP A 594    3536   3077   3491   -207   -123    433       O
ATOM   1573  CB  ASP A 594      21.409  11.909  88.143  1.00 26.02           C
ANISOU 1573  CB  ASP A 594    3316   2893   3678   -104      28    227       C
ATOM   1574  CG  ASP A 594      20.158  11.698  87.293  1.00 27.94           C
ANISOU 1574  CG  ASP A 594    3320   3462   3836   -248     24    205       C
ATOM   1575  OD1 ASP A 594      19.200  12.497  87.384  1.00 29.49           O
ANISOU 1575  OD1 ASP A 594    3488   3625   4092   -107      -8    359       O
ATOM   1576  OD2 ASP A 594      20.100  10.701  86.573  1.00 30.04           O
ANISOU 1576  OD2 ASP A 594    3527   4103   3786     62     64    -73       O
ATOM   1577  N   ALA A 595      23.658  14.827  88.873  1.00 23.58           N
ANISOU 1577  N   ALA A 595    3020   2665   3274   -129    -65    383       N
ATOM   1578  CA  ALA A 595      24.601  15.336  89.833  1.00 24.45           C
ANISOU 1578  CA  ALA A 595    3147   2911   3233   -117   -137    381       C
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ATOM   1579  C   ALA A 595      24.059  16.537  90.580  1.00 25.46           C
ANISOU 1579  C   ALA A 595    3060   3203   3410    -98     17    165       C
ATOM   1580  O   ALA A 595      23.307  17.328  89.966  1.00 27.24           O
ANISOU 1580  O   ALA A 595    3680   3042   3627   -125    -35    377       O
ATOM   1581  CB  ALA A 595      25.823  15.778  88.991  1.00 23.95           C
ANISOU 1581  CB  ALA A 595    2852   2904   3344    -40   -101     74       C
ATOM   1582  N   PRO A 596      24.375  16.744  91.844  1.00 26.95           N
ANISOU 1582  N   PRO A 596    3555   3310   3376   -124     30    231       N
ATOM   1583  CA  PRO A 596      23.931  17.860  92.645  1.00 27.99           C
ANISOU 1583  CA  PRO A 596    3785   3410   3438    -94     23    227       C
ATOM   1584  C   PRO A 596      24.365  19.165  91.958  1.00 27.48           C
ANISOU 1584  C   PRO A 596    3681   3320   3440   -101    -44    185       C
ATOM   1585  O   PRO A 596      25.433  19.130  91.368  1.00 26.15           O
ANISOU 1585  O   PRO A 596    3607   3060   3269    -96   -133    283       O
ATOM   1586  CB  PRO A 596      24.703  17.704  93.953  1.00 29.33           C
ANISOU 1586  CB  PRO A 596    3911   3724   3508     11    -42     93       C
ATOM   1587  CG  PRO A 596      24.951  16.225  94.025  1.00 29.64           C
ANISOU 1587  CG  PRO A 596    4003   3733   3526    -84     35    123       C
ATOM   1588  CD  PRO A 596      25.295  15.831  92.601  1.00 28.42           C
ANISOU 1588  CD  PRO A 596    3716   3566   3515     14    -69     96       C
ATOM   1589  N   LEU A 597      23.524  20.174  91.973  1.00 27.94           N
ANISOU 1589  N   LEU A 597    3929   3250   3436    -51     33    213       N
ATOM   1590  CA  LEU A 597      23.906  21.420  91.243  1.00 27.38           C
ANISOU 1590  CA  LEU A 597    3727   3383   3295    -79     53    277       C
ATOM   1591  C   LEU A 597      24.791  22.293  92.113  1.00 28.84           C
ANISOU 1591  C   LEU A 597    3977   3446   3536   -157     79    201       C
ATOM   1592  O   LEU A 597      24.268  23.207  92.758  1.00 29.55           O
ANISOU 1592  O   LEU A 597    4210   3436   3584   -201    165    175       O
ATOM   1593  CB  LEU A 597      22.596  22.126  90.814  1.00 25.56           C
ANISOU 1593  CB  LEU A 597    3600   3108   3003   -102    223    184       C
ATOM   1594  CG  LEU A 597      21.613  21.275  90.017  1.00 25.30           C
ANISOU 1594  CG  LEU A 597    3413   3191   3009     42    160    174       C
ATOM   1595  CD1 LEU A 597      20.386  22.064  89.594  1.00 23.99           C
ANISOU 1595  CD1 LEU A 597    3367   2805   2944    -20    230    185       C
ATOM   1596  CD2 LEU A 597      22.207  20.601  88.769  1.00 24.88           C
ANISOU 1596  CD2 LEU A 597    3302   2962   3190    169    113    120       C
ATOM   1597  N   ASP A 598      26.090  21.974  92.163  1.00 29.04           N
ANISOU 1597  N   ASP A 598    3977   3497   3560   -191     14    369       N
ATOM   1598  CA  ASP A 598      26.990  22.694  93.045  1.00 31.19           C
ANISOU 1598  CA  ASP A 598    3988   4002   3862   -191    -48    194       C
ATOM   1599  C   ASP A 598      28.111  23.413  92.290  1.00 29.95           C
ANISOU 1599  C   ASP A 598    3848   3913   3620   -147    -65    214       C
ATOM   1600  O   ASP A 598      29.121  23.819  92.878  1.00 31.27           O
ANISOU 1600  O   ASP A 598    4012   4046   3825   -244   -108    309       O
ATOM   1601  CB  ASP A 598      27.572  21.752  94.100  1.00 32.87           C
ANISOU 1601  CB  ASP A 598    4345   4096   4047    -52    -63    262       C
ATOM   1602  CG  ASP A 598      28.265  20.527  93.570  1.00 35.53           C
ANISOU 1602  CG  ASP A 598    4633   4443   4423     47     15     30       C
ATOM   1603  OD1 ASP A 598      28.549  20.335  92.374  1.00 34.43           O
ANISOU 1603  OD1 ASP A 598    4502   4297   4285     19    -53    249       O
ATOM   1604  OD2 ASP A 598      28.529  19.643  94.444  1.00 37.50           O
ANISOU 1604  OD2 ASP A 598    4992   4669   4588    135    -79    138       O
ATOM   1605  N   PHE A 599      27.917  23.551  90.992  1.00 26.85           N
ANISOU 1605  N   PHE A 599    3225   3441   3536   -271    -83    251       N
ATOM   1606  CA  PHE A 599      28.898  24.313  90.190  1.00 24.83           C
ANISOU 1606  CA  PHE A 599    3098   3226   3109   -128   -149    148       C
ATOM   1607  C   PHE A 599      28.790  25.772  90.612  1.00 25.16           C
ANISOU 1607  C   PHE A 599    3151   3265   3146    -82    -21    159       C
ATOM   1608  O   PHE A 599      27.858  26.255  91.265  1.00 25.44           O
ANISOU 1608  O   PHE A 599    3136   3311   3220   -258     27    124       O
ATOM   1609  CB  PHE A 599      28.581  24.102  88.707  1.00 23.88           C
ANISOU 1609  CB  PHE A 599    3038   2995   3041    -53     54    167       C
ATOM   1610  CG  PHE A 599      27.157  24.337  88.304  1.00 23.04           C
ANISOU 1610  CG  PHE A 599    3002   2703   3048   -134     37    107       C
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ATOM   1611  CD1 PHE A 599      26.700  25.624  88.119  1.00 22.28           C
ANISOU 1611  CD1 PHE A 599    2986   2648   2832   -161      6    225       C
ATOM   1612  CD2 PHE A 599      26.248  23.294  88.072  1.00 21.80           C
ANISOU 1612  CD2 PHE A 599    2787   2692   2805   -102    -18    102       C
ATOM   1613  CE1 PHE A 599      25.409  25.882  87.742  1.00 22.53           C
ANISOU 1613  CE1 PHE A 599    2902   2495   3162    -98     48     89       C
ATOM   1614  CE2 PHE A 599      24.959  23.554  87.677  1.00 21.61           C
ANISOU 1614  CE2 PHE A 599    2819   2598   2793     17    167     58       C
ATOM   1615  CZ  PHE A 599      24.500  24.850  87.490  1.00 22.64           C
ANISOU 1615  CZ  PHE A 599    3010   2566   3024   -119    -25     95       C
ATOM   1616  N   ASP A 600      29.798  26.540  90.164  1.00 24.19           N
ANISOU 1616  N   ASP A 600    3133   3051   3009   -160     11    107       N
ATOM   1617  CA  ASP A 600      29.844  27.974  90.466  1.00 25.05           C
ANISOU 1617  CA  ASP A 600    3165   3116   3237    -82     89     28       C
ATOM   1618  C   ASP A 600      30.354  28.804  89.316  1.00 23.68           C
ANISOU 1618  C   ASP A 600    3167   2819   3013      3    -47    -52       C
ATOM   1619  O   ASP A 600      30.542  28.313  88.214  1.00 21.71           O
ANISOU 1619  O   ASP A 600    2866   2354   3030   -112    188     21       O
ATOM   1620  CB  ASP A 600      30.720  28.231  91.701  1.00 26.96           C
ANISOU 1620  CB  ASP A 600    3507   3477   3260   -144    -28     64       C
ATOM   1621  CG  ASP A 600      32.153  27.782  91.458  1.00 29.38           C
ANISOU 1621  CG  ASP A 600    3562   3804   3796    -31    -28    -17       C
ATOM   1622  OD1 ASP A 600      32.679  27.806  90.322  1.00 27.07           O
ANISOU 1622  OD1 ASP A 600    3206   3273   3808   -335   -116    151       O
ATOM   1623  OD2 ASP A 600      32.835  27.340  92.425  1.00 33.08           O
ANISOU 1623  OD2 ASP A 600    4285   4283   4001    -63   -211    224       O
ATOM   1624  N   TYR A 601      30.623  30.104  89.581  1.00 23.00           N
ANISOU 1624  N   TYR A 601    2881   2784   3074   -181      6    -13       N
ATOM   1625  CA  TYR A 601      30.998  30.987  88.477  1.00 23.93           C
ANISOU 1625  CA  TYR A 601    3108   2869   3115    -23    112      4       C
ATOM   1626  C   TYR A 601      32.373  30.687  87.901  1.00 22.53           C
ANISOU 1626  C   TYR A 601    2963   2527   3070   -121     -1    -65       C
ATOM   1627  O   TYR A 601      32.586  31.070  86.749  1.00 22.09           O
ANISOU 1627  O   TYR A 601    2989   2358   3045   -232   -155   -181       O
ATOM   1628  CB  TYR A 601      30.915  32.464  88.854  1.00 25.47           C
ANISOU 1628  CB  TYR A 601    3374   2902   3402     58    169    -11       C
ATOM   1629  CG  TYR A 601      32.106  32.960  89.642  1.00 27.42           C
ANISOU 1629  CG  TYR A 601    3456   3295   3669     53     74   -101       C
ATOM   1630  CD1 TYR A 601      33.002  33.759  88.923  1.00 28.68           C
ANISOU 1630  CD1 TYR A 601    3624   3501   3772    -29    125    -38       C
ATOM   1631  CD2 TYR A 601      32.356  32.704  90.971  1.00 27.34           C
ANISOU 1631  CD2 TYR A 601    3461   3216   3713    -24     49    -77       C
ATOM   1632  CE1 TYR A 601      34.127  34.265  89.545  1.00 31.22           C
ANISOU 1632  CE1 TYR A 601    3922   3822   4117    -95    -46    -82       C
ATOM   1633  CE2 TYR A 601      33.486  33.223  91.622  1.00 30.06           C
ANISOU 1633  CE2 TYR A 601    3700   3660   4061    -59    -82   -168       C
ATOM   1634  CZ  TYR A 601      34.345  34.003  90.870  1.00 31.10           C
ANISOU 1634  CZ  TYR A 601    3948   3810   4059   -102    -12    -80       C
ATOM   1635  OH  TYR A 601      35.489  34.534  91.430  1.00 34.40           O
ANISOU 1635  OH  TYR A 601    4128   4249   4695   -335    -50   -160       O
ATOM   1636  N   LYS A 602      33.235  30.034  88.683  1.00 22.59           N
ANISOU 1636  N   LYS A 602    2780   2694   3110    -50     15    -34       N
ATOM   1637  CA  LYS A 602      34.536  29.637  88.115  1.00 23.43           C
ANISOU 1637  CA  LYS A 602    2910   2822   3171    -66    -34    -87       C
ATOM   1638  C   LYS A 602      34.320  28.485  87.131  1.00 21.11           C
ANISOU 1638  C   LYS A 602    2551   2625   2844    -32    -93    124       C
ATOM   1639  O   LYS A 602      34.974  28.404  86.096  1.00 20.00           O
ANISOU 1639  O   LYS A 602    2793   2215   2593   -110   -270    161       O
ATOM   1640  CB  LYS A 602      35.501  29.259  89.238  1.00 25.08           C
ANISOU 1640  CB  LYS A 602    3216   3205   3108     57    -82     42       C
ATOM   1641  CG  LYS A 602      35.763  30.422  90.178  1.00 28.29           C
ANISOU 1641  CG  LYS A 602    3679   3448   3622    -80     -6   -182       C
ATOM   1642  CD  LYS A 602      36.742  30.059  91.294  1.00 31.15           C
ANISOU 1642  CD  LYS A 602    3996   3959   3880      6   -124    103       C
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ATOM   1643  CE  LYS A 602      36.820  31.260  92.239  1.00 34.67           C
ANISOU 1643  CE  LYS A 602    4624   4288   4261    -68    -69   -124       C
ATOM   1644  NZ  LYS A 602      37.947  31.103  93.200  1.00 36.24           N
ANISOU 1644  NZ  LYS A 602    4693   4587   4488     -2   -158     -7       N
ATOM   1645  N   ASP A 603      33.376  27.576  87.467  1.00 21.49           N
ANISOU 1645  N   ASP A 603    2627   2580   2958    -40   -213     32       N
ATOM   1646  CA  ASP A 603      33.041  26.540  86.512  1.00 20.70           C
ANISOU 1646  CA  ASP A 603    2503   2580   2783    -64    -94     64       C
ATOM   1647  C   ASP A 603      32.507  27.199  85.242  1.00 19.84           C
ANISOU 1647  C   ASP A 603    2374   2362   2802     -9    -39     58       C
ATOM   1648  O   ASP A 603      32.747  26.694  84.168  1.00 20.25           O
ANISOU 1648  O   ASP A 603    2571   2168   2955     22    -34     10       O
ATOM   1649  CB  ASP A 603      31.939  25.602  87.073  1.00 21.75           C
ANISOU 1649  CB  ASP A 603    2753   2565   2946   -117     12     58       C
ATOM   1650  CG  ASP A 603      32.473  24.814  88.259  1.00 24.95           C
ANISOU 1650  CG  ASP A 603    3244   3090   3146     21   -102    103       C
ATOM   1651  OD1 ASP A 603      33.504  24.124  88.067  1.00 26.87           O
ANISOU 1651  OD1 ASP A 603    3238   3253   3718     83   -119    288       O
ATOM   1652  OD2 ASP A 603      31.931  24.832  89.375  1.00 27.25           O
ANISOU 1652  OD2 ASP A 603    3427   3575   3351    -29     37     71       O
ATOM   1653  N   ALA A 604      31.718  28.290  85.353  1.00 19.54           N
ANISOU 1653  N   ALA A 604    2625   2177   2620      7    -79      4       N
ATOM   1654  CA  ALA A 604      31.201  28.929  84.157  1.00 19.18           C
ANISOU 1654  CA  ALA A 604    2317   2340   2631    244     25     23       C
ATOM   1655  C   ALA A 604      32.294  29.466  83.253  1.00 18.27           C
ANISOU 1655  C   ALA A 604    2402   2110   2431    113    -28     -5       C
ATOM   1656  O   ALA A 604      32.274  29.280  82.024  1.00 17.93           O
ANISOU 1656  O   ALA A 604    2357   2005   2452      9   -136     10       O
ATOM   1657  CB  ALA A 604      30.227  30.061  84.549  1.00 18.43           C
ANISOU 1657  CB  ALA A 604    2495   2034   2473    172    217    -85       C
ATOM   1658  N   ILE A 605      33.357  30.040  83.881  1.00 18.09           N
ANISOU 1658  N   ILE A 605    2206   2018   2649     84   -200    101       N
ATOM   1659  CA  ILE A 605      34.524  30.487  83.090  1.00 20.05           C
ANISOU 1659  CA  ILE A 605    2547   2479   2593    -41    -65     99       C
ATOM   1660  C   ILE A 605      35.181  29.333  82.349  1.00 20.12           C
ANISOU 1660  C   ILE A 605    2441   2666   2537    -33    -44     42       C
ATOM   1661  O   ILE A 605      35.406  29.342  81.123  1.00 19.13           O
ANISOU 1661  O   ILE A 605    2040   2732   2496    -99    -53    308       O
ATOM   1662  CB  ILE A 605      35.566  31.179  84.004  1.00 22.12           C
ANISOU 1662  CB  ILE A 605    2722   2902   2781    -53   -161    -18       C
ATOM   1663  CG1 ILE A 605      34.967  32.459  84.578  1.00 23.89           C
ANISOU 1663  CG1 ILE A 605    3070   2951   3055      7   -153    -50       C
ATOM   1664  CG2 ILE A 605      36.839  31.425  83.206  1.00 22.71           C
ANISOU 1664  CG2 ILE A 605    2780   2808   3039   -145    -60     34       C
ATOM   1665  CD1 ILE A 605      35.732  32.980  85.815  1.00 25.66           C
ANISOU 1665  CD1 ILE A 605    3420   3243   3087    -53   -191   -125       C
ATOM   1666  N   ARG A 606      35.368  28.196  83.040  1.00 20.12           N
ANISOU 1666  N   ARG A 606    2448   2560   2637    -79    -51     69       N
ATOM   1667  CA  ARG A 606      35.949  27.000  82.408  1.00 20.36           C
ANISOU 1667  CA  ARG A 606    2577   2493   2667      9    -50    121       C
ATOM   1668  C   ARG A 606      35.010  26.402  81.374  1.00 19.06           C
ANISOU 1668  C   ARG A 606    2646   2122   2474    113    -19    254       C
ATOM   1669  O   ARG A 606      35.447  25.822  80.366  1.00 19.14           O
ANISOU 1669  O   ARG A 606    2476   2306   2493     98    -42    176       O
ATOM   1670  CB  ARG A 606      36.295  25.912  83.473  1.00 22.72           C
ANISOU 1670  CB  ARG A 606    2998   2540   3096    272    -55    189       C
ATOM   1671  CG  ARG A 606      37.308  26.410  84.479  1.00 26.58           C
ANISOU 1671  CG  ARG A 606    3415   3256   3430     66   -151     11       C
ATOM   1672  CD  ARG A 606      38.035  25.267  85.256  1.00 31.19           C
ANISOU 1672  CD  ARG A 606    3774   3958   4120    416   -263    239       C
ATOM   1673  NE  ARG A 606      38.633  25.996  86.406  1.00 36.26           N
ANISOU 1673  NE  ARG A 606    4700   4591   4486     44   -222    -63       N
ATOM   1674  CZ  ARG A 606      38.021  26.191  87.579  1.00 38.29           C
ANISOU 1674  CZ  ARG A 606    4854   4946   4750    102      8    -24       C
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ATOM   1675  NH1 ARG A 606      36.817  25.729  87.869  1.00 37.81           N
ANISOU 1675  NH1 ARG A 606     4845   4766   4756     88    -69     72       N
ATOM   1676  NH2 ARG A 606      38.655  26.909  88.513  1.00 40.36           N
ANISOU 1676  NH2 ARG A 606     5115   5185   5034     24   -103   -129       N
ATOM   1677  N   MET A 607      33.698  26.515  81.636  1.00 18.65           N
ANISOU 1677  N   MET A 607     2407   2017   2662    -87   -177    122       N
ATOM   1678  CA  MET A 607      32.727  25.913  80.700  1.00 17.45           C
ANISOU 1678  CA  MET A 607     2118   2046   2467     66    -29    -52       C
ATOM   1679  C   MET A 607      32.860  26.493  79.316  1.00 17.15           C
ANISOU 1679  C   MET A 607     2198   1824   2492     20    -17    -29       C
ATOM   1680  O   MET A 607      32.678  25.805  78.280  1.00 17.55           O
ANISOU 1680  O   MET A 607     2300   1799   2569    195   -146     14       O
ATOM   1681  CB  MET A 607      31.296  26.054  81.261  1.00 17.74           C
ANISOU 1681  CB  MET A 607     2194   2041   2506     17    -12    -50       C
ATOM   1682  CG  MET A 607      30.294  25.283  80.411  1.00 18.24           C
ANISOU 1682  CG  MET A 607     2330   1868   2732     14    -22    -86       C
ATOM   1683  SD  MET A 607      30.433  23.522  80.870  1.00 21.00           S
ANISOU 1683  SD  MET A 607     2754   1772   3455     20    274     11       S
ATOM   1684  CE  MET A 607      28.922  22.888  80.130  1.00 23.17           C
ANISOU 1684  CE  MET A 607     3229   2264   3312   -110     -4    -70       C
ATOM   1685  N   ARG A 608      33.029  27.838  79.234  1.00 16.78           N
ANISOU 1685  N   ARG A 608     2217   1769   2391   -179    -19     49       N
ATOM   1686  CA  ARG A 608      33.181  28.429  77.908  1.00 17.63           C
ANISOU 1686  CA  ARG A 608     2363   1974   2360     30     30    -43       C
ATOM   1687  C   ARG A 608      34.321  27.799  77.119  1.00 17.62           C
ANISOU 1687  C   ARG A 608     2356   1929   2408    -79    -55     61       C
ATOM   1688  O   ARG A 608      34.190  27.502  75.925  1.00 17.32           O
ANISOU 1688  O   ARG A 608     2299   1917   2366    252      3     66       O
ATOM   1689  CB  ARG A 608      33.449  29.942  77.991  1.00 17.88           C
ANISOU 1689  CB  ARG A 608     2112   2023   2658   -163     54   -138       C
ATOM   1690  CG  ARG A 608      32.229  30.739  78.460  1.00 18.98           C
ANISOU 1690  CG  ARG A 608     2551   1958   2703    128    -14     11       C
ATOM   1691  CD  ARG A 608      32.666  32.253  78.576  1.00 17.55           C
ANISOU 1691  CD  ARG A 608     2249   1946   2474    -71    193   -106       C
ATOM   1692  NE  ARG A 608      31.394  32.915  78.980  1.00 17.14           N
ANISOU 1692  NE  ARG A 608     2186   1846   2482     97   -144    -33       N
ATOM   1693  CZ  ARG A 608      30.504  33.396  78.114  1.00 15.88           C
ANISOU 1693  CZ  ARG A 608     2051   1640   2343     97    109     27       C
ATOM   1694  NH1 ARG A 608      30.772  33.443  76.823  1.00 15.44           N
ANISOU 1694  NH1 ARG A 608     2086   1450   2331    -66     77     64       N
ATOM   1695  NH2 ARG A 608      29.340  33.848  78.621  1.00 16.41           N
ANISOU 1695  NH2 ARG A 608     1942   1619   2673     98    179    -61       N
ATOM   1696  N   ARG A 609      35.453  27.620  77.789  1.00 18.06           N
ANISOU 1696  N   ARG A 609     2279   2080   2503     -8     18    -48       N
ATOM   1697  CA  ARG A 609      36.611  27.001  77.142  1.00 17.41           C
ANISOU 1697  CA  ARG A 609     2022   2049   2543     13     56      1       C
ATOM   1698  C   ARG A 609      36.359  25.524  76.856  1.00 17.72           C
ANISOU 1698  C   ARG A 609     2243   2089   2400    -52     49     16       C
ATOM   1699  O   ARG A 609      36.785  25.068  75.798  1.00 17.83           O
ANISOU 1699  O   ARG A 609     2305   1896   2575    -72     73   -206       O
ATOM   1700  CB  ARG A 609      37.832  27.155  78.056  1.00 18.95           C
ANISOU 1700  CB  ARG A 609     2357   2325   2517     51    -52     31       C
ATOM   1701  CG  ARG A 609      38.083  28.575  78.532  1.00 21.70           C
ANISOU 1701  CG  ARG A 609     2856   2580   2809   -112     68    -75       C
ATOM   1702  CD  ARG A 609      38.122  29.614  77.417  1.00 21.87           C
ANISOU 1702  CD  ARG A 609     2675   2615   3020    106     13     73       C
ATOM   1703  NE  ARG A 609      39.401  29.723  76.724  1.00 24.82           N
ANISOU 1703  NE  ARG A 609     2951   3140   3338    -90     75    -19       N
ATOM   1704  CZ  ARG A 609      39.663  30.813  75.980  1.00 25.69           C
ANISOU 1704  CZ  ARG A 609     3153   3218   3391     19     52     56       C
ATOM   1705  NH1 ARG A 609      40.843  30.889  75.381  1.00 26.94           N
ANISOU 1705  NH1 ARG A 609     3289   3403   3543   -132    194    -78       N
ATOM   1706  NH2 ARG A 609      38.761  31.798  75.850  1.00 25.09           N
ANISOU 1706  NH2 ARG A 609     3025   3077   3430    -96    172     64       N
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ATOM   1707  N   PHE A 610      35.615  24.839  77.721  1.00 17.97           N
ANISOU 1707  N   PHE A 610    2169   2177   2481    -42     71    116       N
ATOM   1708  CA  PHE A 610      35.353  23.406  77.523  1.00 17.48           C
ANISOU 1708  CA  PHE A 610    2024   2123   2495    162     75     21       C
ATOM   1709  C   PHE A 610      34.494  23.220  76.298  1.00 17.42           C
ANISOU 1709  C   PHE A 610    2114   2179   2325     66    201     -2       C
ATOM   1710  O   PHE A 610      34.816  22.420  75.417  1.00 18.23           O
ANISOU 1710  O   PHE A 610    2474   2083   2370    229    142     65       O
ATOM   1711  CB  PHE A 610      34.683  22.863  78.783  1.00 18.11           C
ANISOU 1711  CB  PHE A 610    2222   2089   2570    217    122     94       C
ATOM   1712  CG  PHE A 610      34.227  21.417  78.689  1.00 18.67           C
ANISOU 1712  CG  PHE A 610    2564   2220   2310    -39     55    219       C
ATOM   1713  CD1 PHE A 610      35.118  20.454  78.281  1.00 20.71           C
ANISOU 1713  CD1 PHE A 610    2821   2309   2737     98     24    157       C
ATOM   1714  CD2 PHE A 610      32.915  21.063  79.003  1.00 21.16           C
ANISOU 1714  CD2 PHE A 610    2602   2602   2834   -148     56    104       C
ATOM   1715  CE1 PHE A 610      34.719  19.116  78.219  1.00 21.69           C
ANISOU 1715  CE1 PHE A 610    2966   2382   2894     32    -56    122       C
ATOM   1716  CE2 PHE A 610      32.547  19.718  78.977  1.00 22.54           C
ANISOU 1716  CE2 PHE A 610    3038   2531   2997    -67    238     29       C
ATOM   1717  CZ  PHE A 610      33.426  18.739  78.552  1.00 21.82           C
ANISOU 1717  CZ  PHE A 610    2836   2503   2951     73     43    209       C
ATOM   1718  N   ILE A 611      33.380  23.998  76.222  1.00 16.24           N
ANISOU 1718  N   ILE A 611    2012   1977   2182    127     16    228       N
ATOM   1719  CA  ILE A 611      32.527  23.864  75.035  1.00 16.24           C
ANISOU 1719  CA  ILE A 611    1939   1952   2280    201     12    -37       C
ATOM   1720  C   ILE A 611      33.310  24.212  73.785  1.00 16.58           C
ANISOU 1720  C   ILE A 611    2108   1858   2332    115     30    -64       C
ATOM   1721  O   ILE A 611      33.189  23.530  72.756  1.00 17.64           O
ANISOU 1721  O   ILE A 611    2382   2036   2285    181     -4    -69       O
ATOM   1722  CB  ILE A 611      31.255  24.731  75.132  1.00 15.45           C
ANISOU 1722  CB  ILE A 611    1902   1920   2050    285    104   -116       C
ATOM   1723  CG1 ILE A 611      30.431  24.331  76.354  1.00 16.00           C
ANISOU 1723  CG1 ILE A 611    1929   2044   2105    247     56    -62       C
ATOM   1724  CG2 ILE A 611      30.424  24.655  73.846  1.00 16.68           C
ANISOU 1724  CG2 ILE A 611    2073   2138   2127     41     70    -19       C
ATOM   1725  CD1 ILE A 611      29.280  25.311  76.605  1.00 16.86           C
ANISOU 1725  CD1 ILE A 611    2262   2219   1925    401    -30   -205       C
ATOM   1726  N   ALA A 612      34.115  25.268  73.772  1.00 18.62           N
ANISOU 1726  N   ALA A 612    2225   2017   2834    152    170    -39       N
ATOM   1727  CA  ALA A 612      34.911  25.624  72.624  1.00 18.38           C
ANISOU 1727  CA  ALA A 612    2398   2081   2504     55     68    -93       C
ATOM   1728  C   ALA A 612      35.832  24.451  72.239  1.00 19.28           C
ANISOU 1728  C   ALA A 612    2371   2340   2613    185     70    -14       C
ATOM   1729  O   ALA A 612      35.929  24.157  71.030  1.00 19.78           O
ANISOU 1729  O   ALA A 612    2372   2552   2594    143    312     52       O
ATOM   1730  CB  ALA A 612      35.736  26.885  72.841  1.00 19.07           C
ANISOU 1730  CB  ALA A 612    2617   2230   2400   -100     30    -45       C
ATOM   1731  N   HIS A 613      36.474  23.821  73.221  1.00 19.98           N
ANISOU 1731  N   HIS A 613    2309   2476   2806    124      9     62       N
ATOM   1732  CA  HIS A 613      37.329  22.651  72.937  1.00 20.47           C
ANISOU 1732  CA  HIS A 613    2369   2469   2941     18     80    -62       C
ATOM   1733  C   HIS A 613      36.547  21.510  72.290  1.00 21.13           C
ANISOU 1733  C   HIS A 613    2664   2544   2821     -1    -62    -23       C
ATOM   1734  O   HIS A 613      37.060  20.814  71.381  1.00 21.74           O
ANISOU 1734  O   HIS A 613    2330   2938   2991     14     83     17       O
ATOM   1735  CB  HIS A 613      37.903  22.187  74.295  1.00 22.31           C
ANISOU 1735  CB  HIS A 613    2631   2841   3003     47     14   -116       C
ATOM   1736  CG  HIS A 613      38.624  20.871  74.229  1.00 24.90           C
ANISOU 1736  CG  HIS A 613    3020   3051   3390    203    -67    -22       C
ATOM   1737  ND1 HIS A 613      39.879  20.744  73.679  1.00 27.12           N
ANISOU 1737  ND1 HIS A 613    3270   3437   3598    175    104    -32       N
ATOM   1738  CD2 HIS A 613      38.217  19.650  74.631  1.00 26.89           C
ANISOU 1738  CD2 HIS A 613    3397   3212   3608    156    -67    101       C
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ATOM   1739  CE1 HIS A 613      40.233  19.464  73.770  1.00 27.29           C
ANISOU 1739  CE1 HIS A 613    3385   3415   3569    128     -5    -39       C
ATOM   1740  NE2 HIS A 613      39.255  18.777  74.316  1.00 28.03           N
ANISOU 1740  NE2 HIS A 613    3602   3425   3622    209    134     33       N
ATOM   1741  N   LEU A 614      35.327  21.253  72.788  1.00 19.66           N
ANISOU 1741  N   LEU A 614    2392   2269   2811     80   -163     19       N
ATOM   1742  CA  LEU A 614      34.491  20.168  72.213  1.00 20.01           C
ANISOU 1742  CA  LEU A 614    2508   2301   2793     35    128   -122       C
ATOM   1743  C   LEU A 614      34.231  20.439  70.750  1.00 19.65           C
ANISOU 1743  C   LEU A 614    2353   2291   2821    107     89    -76       C
ATOM   1744  O   LEU A 614      34.239  19.536  69.893  1.00 22.24           O
ANISOU 1744  O   LEU A 614    2787   2573   3090    197    110   -310       O
ATOM   1745  CB  LEU A 614      33.169  19.989  72.985  1.00 19.74           C
ANISOU 1745  CB  LEU A 614    2497   2272   2730     44     63    -50       C
ATOM   1746  CG  LEU A 614      33.308  19.558  74.459  1.00 19.67           C
ANISOU 1746  CG  LEU A 614    2396   2295   2784    215     83    -35       C
ATOM   1747  CD1 LEU A 614      31.949  19.510  75.146  1.00 19.67           C
ANISOU 1747  CD1 LEU A 614    2708   2145   2621    -57    207     10       C
ATOM   1748  CD2 LEU A 614      33.944  18.152  74.506  1.00 20.94           C
ANISOU 1748  CD2 LEU A 614    3022   2012   2923     15    120     40       C
ATOM   1749  N   ILE A 615      33.965  21.698  70.391  1.00 18.12           N
ANISOU 1749  N   ILE A 615    2168   2250   2465    -32    144     31       N
ATOM   1750  CA  ILE A 615      33.720  22.059  68.995  1.00 18.12           C
ANISOU 1750  CA  ILE A 615    2398   2077   2409     99     85    -72       C
ATOM   1751  C   ILE A 615      34.967  21.831  68.146  1.00 20.48           C
ANISOU 1751  C   ILE A 615    2572   2621   2588    -51    178    -32       C
ATOM   1752  O   ILE A 615      34.860  21.203  67.080  1.00 22.69           O
ANISOU 1752  O   ILE A 615    2927   2694   3001    -15    307   -278       O
ATOM   1753  CB  ILE A 615      33.263  23.546  68.925  1.00 18.30           C
ANISOU 1753  CB  ILE A 615    2496   2017   2441     25     86   -122       C
ATOM   1754  CG1 ILE A 615      31.880  23.653  69.547  1.00 17.52           C
ANISOU 1754  CG1 ILE A 615    2422   1987   2248    -41    134   -141       C
ATOM   1755  CG2 ILE A 615      33.228  23.975  67.481  1.00 20.24           C
ANISOU 1755  CG2 ILE A 615    2754   2517   2418     88     45   -112       C
ATOM   1756  CD1 ILE A 615      31.356  25.064  69.831  1.00 18.55           C
ANISOU 1756  CD1 ILE A 615    2472   2053   2523     56     20   -102       C
ATOM   1757  N   LEU A 616      36.102  22.327  68.598  1.00 21.45           N
ANISOU 1757  N   LEU A 616    2581   2872   2696    -49    166   -217       N
ATOM   1758  CA  LEU A 616      37.342  22.218  67.795  1.00 22.75           C
ANISOU 1758  CA  LEU A 616    2616   3016   3014     95    242   -179       C
ATOM   1759  C   LEU A 616      37.803  20.779  67.676  1.00 24.30           C
ANISOU 1759  C   LEU A 616    3075   3016   3144     87    131   -173       C
ATOM   1760  O   LEU A 616      38.525  20.439  66.709  1.00 27.12           O
ANISOU 1760  O   LEU A 616    3319   3620   3367    101    421   -246       O
ATOM   1761  CB  LEU A 616      38.463  23.090  68.401  1.00 24.20           C
ANISOU 1761  CB  LEU A 616    2926   3134   3137     24     79    -87       C
ATOM   1762  CG  LEU A 616      38.143  24.601  68.424  1.00 23.96           C
ANISOU 1762  CG  LEU A 616    2932   3094   3077    -67     43    -97       C
ATOM   1763  CD1 LEU A 616      39.340  25.345  69.003  1.00 24.71           C
ANISOU 1763  CD1 LEU A 616    2827   3304   3257    -99    143    -95       C
ATOM   1764  CD2 LEU A 616      37.687  25.127  67.070  1.00 24.18           C
ANISOU 1764  CD2 LEU A 616    2823   3353   3010   -112    183    -93       C
ATOM   1765  N   THR A 617      37.465  19.938  68.624  1.00 24.70           N
ANISOU 1765  N   THR A 617    3019   3206   3160    143     74    -76       N
ATOM   1766  CA  THR A 617      37.874  18.535  68.575  1.00 26.86           C
ANISOU 1766  CA  THR A 617    3444   3234   3529    140      6    -81       C
ATOM   1767  C   THR A 617      36.800  17.638  67.990  1.00 27.41           C
ANISOU 1767  C   THR A 617    3561   3318   3537    100    -42    -81       C
ATOM   1768  O   THR A 617      36.922  16.401  68.061  1.00 27.99           O
ANISOU 1768  O   THR A 617    3683   3287   3663    205     22     49       O
ATOM   1769  CB  THR A 617      38.363  18.063  69.958  1.00 27.91           C
ANISOU 1769  CB  THR A 617    3614   3416   3574     44      0     33       C
ATOM   1770  OG1 THR A 617      37.296  18.211  70.880  1.00 27.25           O
ANISOU 1770  OG1 THR A 617    3519   3134   3702    273    -46    -40       O
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ATOM   1771  CG2 THR A 617      39.576  18.891  70.379  1.00 28.06           C
ANISOU 1771  CG2 THR A 617    3685   3282   3695    105    -26    -73       C
ATOM   1772  N   ASP A 618      35.777  18.223  67.367  1.00 26.05           N
ANISOU 1772  N   ASP A 618    3386   3188   3323    184    145   -162       N
ATOM   1773  CA  ASP A 618      34.752  17.468  66.657  1.00 26.29           C
ANISOU 1773  CA  ASP A 618    3300   3247   3443    103    141    -90       C
ATOM   1774  C   ASP A 618      34.217  16.378  67.564  1.00 26.42           C
ANISOU 1774  C   ASP A 618    3335   3310   3394     -1     36    -48       C
ATOM   1775  O   ASP A 618      34.106  15.184  67.231  1.00 28.47           O
ANISOU 1775  O   ASP A 618    3766   3429   3621     97    265   -221       O
ATOM   1776  CB  ASP A 618      35.387  16.865  65.402  1.00 27.42           C
ANISOU 1776  CB  ASP A 618    3593   3470   3355     18    124    -86       C
ATOM   1777  CG  ASP A 618      34.473  16.394  64.307  1.00 29.38           C
ANISOU 1777  CG  ASP A 618    3695   3827   3643     64     20   -170       C
ATOM   1778  OD1 ASP A 618      33.272  16.690  64.259  1.00 28.30           O
ANISOU 1778  OD1 ASP A 618    3575   3617   3561     46     30   -177       O
ATOM   1779  OD2 ASP A 618      35.013  15.712  63.385  1.00 30.41           O
ANISOU 1779  OD2 ASP A 618    3908   3839   3806    114     83   -324       O
ATOM   1780  N   ALA A 619      33.736  16.776  68.731  1.00 26.15           N
ANISOU 1780  N   ALA A 619    3280   3141   3515     -6    105   -129       N
ATOM   1781  CA  ALA A 619      33.275  15.864  69.770  1.00 27.62           C
ANISOU 1781  CA  ALA A 619    3633   3383   3477     81     45    -32       C
ATOM   1782  C   ALA A 619      32.068  15.032  69.419  1.00 27.85           C
ANISOU 1782  C   ALA A 619    3762   3295   3526     73     63   -134       C
ATOM   1783  O   ALA A 619      31.819  14.056  70.136  1.00 28.62           O
ANISOU 1783  O   ALA A 619    4120   3361   3392    -16    121   -227       O
ATOM   1784  CB  ALA A 619      33.022  16.646  71.066  1.00 29.09           C
ANISOU 1784  CB  ALA A 619    4019   3553   3483     52     91    -75       C
ATOM   1785  N   LEU A 620      31.326  15.357  68.371  1.00 26.99           N
ANISOU 1785  N   LEU A 620    3593   3232   3429     44    102   -257       N
ATOM   1786  CA  LEU A 620      30.151  14.556  68.024  1.00 27.73           C
ANISOU 1786  CA  LEU A 620    3608   3365   3564     -6     36   -209       C
ATOM   1787  C   LEU A 620      30.529  13.416  67.070  1.00 30.37           C
ANISOU 1787  C   LEU A 620    4115   3680   3744     20     96   -361       C
ATOM   1788  O   LEU A 620      29.596  12.684  66.711  1.00 31.58           O
ANISOU 1788  O   LEU A 620    4099   3835   4064    -36    218   -362       O
ATOM   1789  CB  LEU A 620      29.050  15.406  67.434  1.00 26.26           C
ANISOU 1789  CB  LEU A 620    3465   3153   3361   -103     93   -317       C
ATOM   1790  CG  LEU A 620      28.679  16.652  68.271  1.00 25.84           C
ANISOU 1790  CG  LEU A 620    3365   3163   3290     44     50   -245       C
ATOM   1791  CD1 LEU A 620      27.702  17.486  67.465  1.00 25.51           C
ANISOU 1791  CD1 LEU A 620    3310   3188   3196   -106      7   -167       C
ATOM   1792  CD2 LEU A 620      28.148  16.243  69.630  1.00 26.24           C
ANISOU 1792  CD2 LEU A 620    3379   3280   3310    -85    -37   -155       C
ATOM   1793  N   LYS A 621      31.796  13.208  66.768  1.00 32.72           N
ANISOU 1793  N   LYS A 621    4175   3990   4266     50     99    -65       N
ATOM   1794  CA  LYS A 621      32.184  12.071  65.922  1.00 36.62           C
ANISOU 1794  CA  LYS A 621    4758   4481   4676    149    201   -311       C
ATOM   1795  C   LYS A 621      31.137  11.666  64.901  1.00 38.99           C
ANISOU 1795  C   LYS A 621    4958   4897   4960     54     19   -146       C
ATOM   1796  O   LYS A 621      31.105  10.428  64.598  1.00 41.65           O
ANISOU 1796  O   LYS A 621    5441   4896   5488     39     90   -189       O
ATOM   1797  CB  LYS A 621      32.540  10.823  66.748  1.00 39.07           C
ANISOU 1797  CB  LYS A 621    5043   4693   5111    159     37    -98       C
ATOM   1798  CG  LYS A 621      31.583  10.196  67.684  1.00 42.00           C
ANISOU 1798  CG  LYS A 621    5286   5345   5328     30    128    -25       C
ATOM   1799  CD  LYS A 621      31.797   8.768  68.147  1.00 44.44           C
ANISOU 1799  CD  LYS A 621    5734   5463   5688     60     47     36       C
ATOM   1800  CE  LYS A 621      30.905   7.777  67.425  1.00 45.57           C
ANISOU 1800  CE  LYS A 621    5760   5741   5813    -48     20     10       C
ATOM   1801  NZ  LYS A 621      31.375   6.374  67.661  1.00 46.21           N
ANISOU 1801  NZ  LYS A 621    5891   5768   5900     -2    -48    -29       N
TER    1802       LYS A 621
ATOM   1803  N   PRO B  20       5.110  13.180  40.537  1.00 61.48           N
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ANISOU 1803  N   PRO B  20     7765   7820   7774     -4     16    -39       N
ATOM   1804  CA  PRO B  20       5.653  13.683  41.845  1.00 61.11           C
ANISOU 1804  CA  PRO B  20     7685   7788   7747     43      9     -2       C
ATOM   1805  C   PRO B  20       6.859  12.823  42.221  1.00 60.40           C
ANISOU 1805  C   PRO B  20     7627   7719   7601      5     48    -25       C
ATOM   1806  O   PRO B  20       7.088  12.459  43.370  1.00 60.60           O
ANISOU 1806  O   PRO B  20     7696   7700   7627     -3     21     21       O
ATOM   1807  N   GLU B  21       7.642  12.514  41.182  1.00 59.31           N
ANISOU 1807  N   GLU B  21     7454   7536   7546     63    -23      2       N
ATOM   1808  CA  GLU B  21       8.823  11.690  41.325  1.00 56.74           C
ANISOU 1808  CA  GLU B  21     7183   7225   7151   -114     12    -50       C
ATOM   1809  C   GLU B  21      10.081  12.447  41.693  1.00 54.30           C
ANISOU 1809  C   GLU B  21     6933   6896   6803     36    102     28       C
ATOM   1810  O   GLU B  21      10.419  12.521  42.878  1.00 55.02           O
ANISOU 1810  O   GLU B  21     6999   7017   6888     13     14    -39       O
ATOM   1811  N   THR B  22      10.789  13.010  40.719  1.00 51.54           N
ANISOU 1811  N   THR B  22     6494   6494   6594     -2    -83   -100       N
ATOM   1812  CA  THR B  22      12.066  13.658  40.960  1.00 48.75           C
ANISOU 1812  CA  THR B  22     6360   6038   6125     63      2    -91       C
ATOM   1813  C   THR B  22      11.996  15.039  41.602  1.00 45.57           C
ANISOU 1813  C   THR B  22     5738   5853   5725     79     31     51       C
ATOM   1814  O   THR B  22      13.004  15.512  42.136  1.00 43.92           O
ANISOU 1814  O   THR B  22     5775   5404   5507    115    143    -37       O
ATOM   1815  CB  THR B  22      12.928  13.823  39.683  1.00 49.62           C
ANISOU 1815  CB  THR B  22     6344   6270   6242     10     12      0       C
ATOM   1816  OG1 THR B  22      12.271  14.675  38.736  1.00 49.60           O
ANISOU 1816  OG1 THR B  22     6338   6290   6217    -68    -66     16       O
ATOM   1817  CG2 THR B  22      13.218  12.478  39.042  1.00 50.11           C
ANISOU 1817  CG2 THR B  22     6447   6295   6298     -2      3    -50       C
ATOM   1818  N   HIS B  23      10.849  15.690  41.493  1.00 43.04           N
ANISOU 1818  N   HIS B  23     5682   5429   5241     -4     35    -57       N
ATOM   1819  CA  HIS B  23      10.705  17.037  42.018  1.00 41.20           C
ANISOU 1819  CA  HIS B  23     5248   5383   5024     14    135    -13       C
ATOM   1820  C   HIS B  23       9.853  17.065  43.283  1.00 38.16           C
ANISOU 1820  C   HIS B  23     4955   4794   4752     12    -43    -40       C
ATOM   1821  O   HIS B  23       9.121  16.125  43.560  1.00 36.19           O
ANISOU 1821  O   HIS B  23     4696   4817   4237     58    125   -171       O
ATOM   1822  CB  HIS B  23      10.117  17.932  40.916  1.00 43.73           C
ANISOU 1822  CB  HIS B  23     5636   5572   5405     81    -69     83       C
ATOM   1823  CG  HIS B  23      11.122  18.006  39.795  1.00 45.32           C
ANISOU 1823  CG  HIS B  23     5754   5826   5639     44     32     60       C
ATOM   1824  ND1 HIS B  23      10.988  17.306  38.613  1.00 45.91           N
ANISOU 1824  ND1 HIS B  23     5844   5796   5803     33    -27    -28       N
ATOM   1825  CD2 HIS B  23      12.289  18.675  39.727  1.00 45.45           C
ANISOU 1825  CD2 HIS B  23     5678   5868   5723     47    -88     35       C
ATOM   1826  CE1 HIS B  23      12.038  17.579  37.860  1.00 46.16           C
ANISOU 1826  CE1 HIS B  23     5833   5845   5861     27    -14     18       C
ATOM   1827  NE2 HIS B  23      12.853  18.398  38.510  1.00 45.79           N
ANISOU 1827  NE2 HIS B  23     5779   5879   5742     73    -56     12       N
ATOM   1828  N   ILE B  24      10.037  18.130  44.055  1.00 35.73           N
ANISOU 1828  N   ILE B  24     4644   4712   4221     46     65     96       N
ATOM   1829  CA  ILE B  24       9.266  18.228  45.309  1.00 34.64           C
ANISOU 1829  CA  ILE B  24     4411   4542   4207     59      2    -16       C
ATOM   1830  C   ILE B  24       8.755  19.636  45.485  1.00 33.36           C
ANISOU 1830  C   ILE B  24     4205   4508   3964    -13     65    -13       C
ATOM   1831  O   ILE B  24       9.443  20.604  45.140  1.00 33.90           O
ANISOU 1831  O   ILE B  24     4417   4464   4000     86    238    -41       O
ATOM   1832  CB  ILE B  24      10.176  17.769  46.473  1.00 34.49           C
ANISOU 1832  CB  ILE B  24     4433   4445   4229     47     -7     34       C
ATOM   1833  CG1 ILE B  24       9.432  17.740  47.820  1.00 34.59           C
ANISOU 1833  CG1 ILE B  24     4397   4470   4275     31     11     -4       C
ATOM   1834  CG2 ILE B  24      11.431  18.624  46.600  1.00 34.31           C
ANISOU 1834  CG2 ILE B  24     4362   4496   4177     83     48     35       C
ATOM   1835  CD1 ILE B  24      10.315  17.225  48.953  1.00 34.94           C
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ANISOU 1835  CD1 ILE B  24     4470   4561   4243    -54    -32      4       C
ATOM   1836  N   ASN B  25       7.552  19.772  46.042  1.00 31.98           N
ANISOU 1836  N   ASN B  25     4085   4308   3759     72    -28      5       N
ATOM   1837  CA  ASN B  25       7.014  21.082  46.374  1.00 31.71           C
ANISOU 1837  CA  ASN B  25     4157   4165   3725    -46    -15     73       C
ATOM   1838  C   ASN B  25       7.301  21.371  47.863  1.00 31.16           C
ANISOU 1838  C   ASN B  25     4094   4041   3705      4     67     41       C
ATOM   1839  O   ASN B  25       7.057  20.526  48.734  1.00 30.08           O
ANISOU 1839  O   ASN B  25     4073   4004   3352    145    -24    -10       O
ATOM   1840  CB  ASN B  25       5.512  21.160  46.129  1.00 33.14           C
ANISOU 1840  CB  ASN B  25     4208   4419   3965     33    -43     23       C
ATOM   1841  CG  ASN B  25       5.198  20.951  44.637  1.00 33.80           C
ANISOU 1841  CG  ASN B  25     4382   4484   3976     27    -34     58       C
ATOM   1842  OD1 ASN B  25       5.366  21.915  43.902  1.00 34.49           O
ANISOU 1842  OD1 ASN B  25     4398   4797   3911     21   -100    212       O
ATOM   1843  ND2 ASN B  25       4.800  19.774  44.226  1.00 33.52           N
ANISOU 1843  ND2 ASN B  25     4360   4642   3736    -70    -90     18       N
ATOM   1844  N   LEU B  26       7.859  22.537  48.128  1.00 29.72           N
ANISOU 1844  N   LEU B  26     3737   4092   3461     10     49     18       N
ATOM   1845  CA  LEU B  26       8.206  22.949  49.479  1.00 29.18           C
ANISOU 1845  CA  LEU B  26     3705   3863   3519    -15     26    -39       C
ATOM   1846  C   LEU B  26       7.736  24.371  49.741  1.00 30.72           C
ANISOU 1846  C   LEU B  26     4018   3969   3687     89     27    -27       C
ATOM   1847  O   LEU B  26       7.687  25.217  48.846  1.00 31.50           O
ANISOU 1847  O   LEU B  26     4314   4057   3598    177    171    -39       O
ATOM   1848  CB  LEU B  26       9.731  22.863  49.685  1.00 28.96           C
ANISOU 1848  CB  LEU B  26     3717   3871   3416     18      0     33       C
ATOM   1849  CG  LEU B  26      10.331  21.453  49.656  1.00 28.32           C
ANISOU 1849  CG  LEU B  26     3564   3813   3382    -41    -20    -55       C
ATOM   1850  CD1 LEU B  26      11.866  21.481  49.715  1.00 29.50           C
ANISOU 1850  CD1 LEU B  26     3586   3992   3629    -51    -21    -27       C
ATOM   1851  CD2 LEU B  26       9.767  20.542  50.729  1.00 29.13           C
ANISOU 1851  CD2 LEU B  26     3629   3955   3484    -52    -64     15       C
ATOM   1852  N   LYS B  27       7.401  24.629  51.014  1.00 29.78           N
ANISOU 1852  N   LYS B  27     3771   3974   3572    -27    -52     -9       N
ATOM   1853  CA  LYS B  27       7.012  25.998  51.363  1.00 30.79           C
ANISOU 1853  CA  LYS B  27     3892   4060   3746     -9    -95    -64       C
ATOM   1854  C   LYS B  27       8.038  26.495  52.384  1.00 29.56           C
ANISOU 1854  C   LYS B  27     3726   3835   3668     24      6   -100       C
ATOM   1855  O   LYS B  27       8.414  25.686  53.235  1.00 29.68           O
ANISOU 1855  O   LYS B  27     3728   3844   3704    -22   -156   -112       O
ATOM   1856  CB  LYS B  27       5.631  26.014  51.972  1.00 32.36           C
ANISOU 1856  CB  LYS B  27     3900   4374   4022    -72   -108     22       C
ATOM   1857  CG  LYS B  27       5.156  27.280  52.653  1.00 35.05           C
ANISOU 1857  CG  LYS B  27     4381   4510   4427     67    -44    -26       C
ATOM   1858  CD  LYS B  27       3.673  27.065  52.992  1.00 36.85           C
ANISOU 1858  CD  LYS B  27     4419   4881   4702     53    -45     13       C
ATOM   1859  CE  LYS B  27       3.416  27.273  54.463  1.00 38.44           C
ANISOU 1859  CE  LYS B  27     4810   5039   4757     68    -37     18       C
ATOM   1860  NZ  LYS B  27       1.957  27.453  54.704  1.00 38.50           N
ANISOU 1860  NZ  LYS B  27     4762   5081   4784    -23     50     -3       N
ATOM   1861  N   VAL B  28       8.462  27.741  52.287  1.00 28.44           N
ANISOU 1861  N   VAL B  28     3494   3850   3460    101     98    -40       N
ATOM   1862  CA  VAL B  28       9.336  28.264  53.341  1.00 28.28           C
ANISOU 1862  CA  VAL B  28     3600   3584   3560    109     12    -89       C
ATOM   1863  C   VAL B  28       8.510  29.348  54.057  1.00 28.57           C
ANISOU 1863  C   VAL B  28     3640   3685   3532    117    141    -49       C
ATOM   1864  O   VAL B  28       7.940  30.162  53.332  1.00 29.58           O
ANISOU 1864  O   VAL B  28     3832   3778   3631    302     89   -128       O
ATOM   1865  CB  VAL B  28      10.636  28.862  52.835  1.00 28.62           C
ANISOU 1865  CB  VAL B  28     3723   3645   3508     26    -11    -37       C
ATOM   1866  CG1 VAL B  28      11.509  29.407  53.974  1.00 28.63           C
ANISOU 1866  CG1 VAL B  28     3864   3620   3394     51    -71     70       C
ATOM   1867  CG2 VAL B  28      11.430  27.758  52.137  1.00 28.83           C
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ANISOU 1867  CG2 VAL B  28     3817   3688   3451    131     38     46       C
ATOM   1868  N   SER B  29       8.475  29.305  55.375  1.00 27.01           N
ANISOU 1868  N   SER B  29     3435   3337   3488     97     26    -78       N
ATOM   1869  CA  SER B  29       7.676  30.330  56.066  1.00 27.64           C
ANISOU 1869  CA  SER B  29     3494   3515   3494     39    146   -118       C
ATOM   1870  C   SER B  29       8.450  30.928  57.238  1.00 27.95           C
ANISOU 1870  C   SER B  29     3356   3719   3545     60     15     -4       C
ATOM   1871  O   SER B  29       9.036  30.132  57.935  1.00 27.98           O
ANISOU 1871  O   SER B  29     3400   3826   3404      5     20     82       O
ATOM   1872  CB  SER B  29       6.434  29.666  56.688  1.00 27.35           C
ANISOU 1872  CB  SER B  29     3348   3631   3414    -28      5   -133       C
ATOM   1873  OG  SER B  29       5.618  30.700  57.245  1.00 28.47           O
ANISOU 1873  OG  SER B  29     3408   3748   3660    108   -222   -241       O
ATOM   1874  N   ASP B  30       8.296  32.232  57.468  1.00 29.97           N
ANISOU 1874  N   ASP B  30     3855   3745   3787     -8     59    -15       N
ATOM   1875  CA  ASP B  30       8.865  32.804  58.687  1.00 31.94           C
ANISOU 1875  CA  ASP B  30     4057   4063   4016     44   -190      1       C
ATOM   1876  C   ASP B  30       7.739  33.119  59.670  1.00 32.68           C
ANISOU 1876  C   ASP B  30     4366   4094   3957    -35    -20    156       C
ATOM   1877  O   ASP B  30       7.947  33.860  60.627  1.00 33.73           O
ANISOU 1877  O   ASP B  30     4556   4160   4100     36   -107     80       O
ATOM   1878  CB  ASP B  30       9.710  34.046  58.429  1.00 32.87           C
ANISOU 1878  CB  ASP B  30     4267   4038   4184     63    -61     43       C
ATOM   1879  CG  ASP B  30       8.915  35.173  57.776  1.00 33.72           C
ANISOU 1879  CG  ASP B  30     4407   4149   4259     55    -90    120       C
ATOM   1880  OD1 ASP B  30       7.684  35.039  57.697  1.00 33.45           O
ANISOU 1880  OD1 ASP B  30     4354   4133   4221    268    -98    101       O
ATOM   1881  OD2 ASP B  30       9.609  36.136  57.394  1.00 34.14           O
ANISOU 1881  OD2 ASP B  30     4575   4060   4337     21   -154    133       O
ATOM   1882  N   GLY B  31       6.523  32.650  59.366  1.00 33.99           N
ANISOU 1882  N   GLY B  31     4279   4372   4263     75    -84    201       N
ATOM   1883  CA  GLY B  31       5.377  32.943  60.232  1.00 35.82           C
ANISOU 1883  CA  GLY B  31     4501   4628   4483    -18     78    107       C
ATOM   1884  C   GLY B  31       4.545  34.087  59.654  1.00 37.63           C
ANISOU 1884  C   GLY B  31     4733   4710   4856     84    -56     16       C
ATOM   1885  O   GLY B  31       3.410  34.293  60.088  1.00 38.14           O
ANISOU 1885  O   GLY B  31     4836   4778   4875    178     65     73       O
ATOM   1886  N   SER B  32       5.075  34.839  58.696  1.00 39.48           N
ANISOU 1886  N   SER B  32     5045   5039   4915     24     53     48       N
ATOM   1887  CA  SER B  32       4.230  35.913  58.137  1.00 41.83           C
ANISOU 1887  CA  SER B  32     5291   5287   5315    138    -36    101       C
ATOM   1888  C   SER B  32       4.388  35.939  56.629  1.00 41.91           C
ANISOU 1888  C   SER B  32     5324   5281   5318     57    -33     44       C
ATOM   1889  O   SER B  32       3.430  36.142  55.889  1.00 42.31           O
ANISOU 1889  O   SER B  32     5320   5338   5418     -4    -88    -18       O
ATOM   1890  CB  SER B  32       4.483  37.238  58.820  1.00 43.48           C
ANISOU 1890  CB  SER B  32     5586   5412   5522     47    -40     17       C
ATOM   1891  OG  SER B  32       5.833  37.625  58.826  1.00 45.44           O
ANISOU 1891  OG  SER B  32     5627   5812   5826     43    -37    128       O
ATOM   1892  N   SER B  33       5.603  35.698  56.179  1.00 41.29           N
ANISOU 1892  N   SER B  33     5337   5177   5173     70    -18     43       N
ATOM   1893  CA  SER B  33       5.909  35.639  54.751  1.00 40.95           C
ANISOU 1893  CA  SER B  33     5275   5148   5135     58    -77    -16       C
ATOM   1894  C   SER B  33       6.145  34.181  54.379  1.00 39.85           C
ANISOU 1894  C   SER B  33     5060   5125   4957     89    -75    -27       C
ATOM   1895  O   SER B  33       6.910  33.481  55.051  1.00 38.57           O
ANISOU 1895  O   SER B  33     4927   5004   4725    -19    -47    -26       O
ATOM   1896  CB  SER B  33       7.114  36.520  54.479  1.00 41.78           C
ANISOU 1896  CB  SER B  33     5333   5254   5287      3    -43     24       C
ATOM   1897  OG  SER B  33       7.800  36.180  53.287  1.00 43.51           O
ANISOU 1897  OG  SER B  33     5620   5484   5429     64     70    -39       O
ATOM   1898  N   GLU B  34       5.421  33.685  53.375  1.00 39.09           N
ANISOU 1898  N   GLU B  34     4914   5033   4906    136    -64     19       N
ATOM   1899  CA  GLU B  34       5.625  32.300  52.943  1.00 39.40           C
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ANISOU 1899  CA  GLU B  34     5037   5061   4872    143    -93     -7       C
ATOM   1900  C   GLU B  34       5.855  32.255  51.441  1.00 38.17           C
ANISOU 1900  C   GLU B  34     4759   4880   4865    143     -9     44       C
ATOM   1901  O   GLU B  34       5.247  33.013  50.670  1.00 37.97           O
ANISOU 1901  O   GLU B  34     4720   4965   4740    183    -64     30       O
ATOM   1902  CB  GLU B  34       4.538  31.363  53.413  1.00 42.32           C
ANISOU 1902  CB  GLU B  34     5384   5292   5403    -37     18     26       C
ATOM   1903  CG  GLU B  34       3.092  31.728  53.153  1.00 45.21           C
ANISOU 1903  CG  GLU B  34     5558   5793   5826     55    -86    -39       C
ATOM   1904  CD  GLU B  34       2.231  31.106  54.254  1.00 47.57           C
ANISOU 1904  CD  GLU B  34     5946   6095   6033    -38     45     64       C
ATOM   1905  OE1 GLU B  34       1.935  31.835  55.239  1.00 49.22           O
ANISOU 1905  OE1 GLU B  34     6208   6370   6124     -7     64    -12       O
ATOM   1906  OE2 GLU B  34       1.882  29.922  54.132  1.00 47.63           O
ANISOU 1906  OE2 GLU B  34     5936   6094   6066     10     45    -17       O
ATOM   1907  N   ILE B  35       6.854  31.475  51.029  1.00 36.43           N
ANISOU 1907  N   ILE B  35     4694   4738   4411    129    -75     44       N
ATOM   1908  CA  ILE B  35       7.209  31.364  49.611  1.00 35.38           C
ANISOU 1908  CA  ILE B  35     4485   4541   4415    115    -44     85       C
ATOM   1909  C   ILE B  35       7.201  29.890  49.233  1.00 33.87           C
ANISOU 1909  C   ILE B  35     4233   4495   4139    141     -1    101       C
ATOM   1910  O   ILE B  35       7.742  29.056  49.957  1.00 32.10           O
ANISOU 1910  O   ILE B  35     4048   4560   3589    101    205    166       O
ATOM   1911  CB  ILE B  35       8.583  31.989  49.305  1.00 35.74           C
ANISOU 1911  CB  ILE B  35     4594   4558   4428     71      9     70       C
ATOM   1912  CG1 ILE B  35       8.655  33.440  49.757  1.00 35.99           C
ANISOU 1912  CG1 ILE B  35     4649   4557   4470     20    -50    107       C
ATOM   1913  CG2 ILE B  35       8.849  31.836  47.813  1.00 35.28           C
ANISOU 1913  CG2 ILE B  35     4494   4515   4395     24     16    108       C
ATOM   1914  CD1 ILE B  35      10.009  34.086  49.738  1.00 37.60           C
ANISOU 1914  CD1 ILE B  35     4766   4690   4831    -38    -50     51       C
ATOM   1915  N   PHE B  36       6.546  29.539  48.130  1.00 33.78           N
ANISOU 1915  N   PHE B  36     4335   4443   4059    122     34    124       N
ATOM   1916  CA  PHE B  36       6.443  28.183  47.636  1.00 34.11           C
ANISOU 1916  CA  PHE B  36     4385   4468   4107     66     50    100       C
ATOM   1917  C   PHE B  36       7.487  27.964  46.537  1.00 33.99           C
ANISOU 1917  C   PHE B  36     4333   4388   4194     96     10     60       C
ATOM   1918  O   PHE B  36       7.753  28.877  45.747  1.00 32.71           O
ANISOU 1918  O   PHE B  36     4170   4417   3843    126    108    -43       O
ATOM   1919  CB  PHE B  36       5.076  27.884  47.022  1.00 36.02           C
ANISOU 1919  CB  PHE B  36     4508   4717   4459     27    -32     23       C
ATOM   1920  CG  PHE B  36       3.984  27.916  48.065  1.00 37.58           C
ANISOU 1920  CG  PHE B  36     4635   4993   4653     18     54     10       C
ATOM   1921  CD1 PHE B  36       3.421  29.125  48.440  1.00 38.57           C
ANISOU 1921  CD1 PHE B  36     4841   5031   4783     50     -2    -21       C
ATOM   1922  CD2 PHE B  36       3.556  26.746  48.651  1.00 38.52           C
ANISOU 1922  CD2 PHE B  36     4818   4985   4834     13     -1     42       C
ATOM   1923  CE1 PHE B  36       2.404  29.155  49.389  1.00 38.81           C
ANISOU 1923  CE1 PHE B  36     4791   5081   4875     15     16    -17       C
ATOM   1924  CE2 PHE B  36       2.540  26.776  49.605  1.00 39.51           C
ANISOU 1924  CE2 PHE B  36     4963   5111   4939     25     77    -31       C
ATOM   1925  CZ  PHE B  36       1.981  27.980  49.968  1.00 39.14           C
ANISOU 1925  CZ  PHE B  36     4847   5070   4955     36     18      9       C
ATOM   1926  N   PHE B  37       8.125  26.806  46.615  1.00 33.20           N
ANISOU 1926  N   PHE B  37     4255   4317   4042     72     31     11       N
ATOM   1927  CA  PHE B  37       9.179  26.480  45.670  1.00 33.43           C
ANISOU 1927  CA  PHE B  37     4142   4413   4149     38     12     38       C
ATOM   1928  C   PHE B  37       8.946  25.074  45.152  1.00 34.30           C
ANISOU 1928  C   PHE B  37     4313   4445   4274     30      3      4       C
ATOM   1929  O   PHE B  37       8.320  24.252  45.809  1.00 35.32           O
ANISOU 1929  O   PHE B  37     4473   4673   4273    -10     46    105       O
ATOM   1930  CB  PHE B  37      10.555  26.496  46.355  1.00 32.86           C
ANISOU 1930  CB  PHE B  37     4077   4273   4135     -8     53     22       C
ATOM   1931  CG  PHE B  37      11.005  27.793  46.939  1.00 32.59           C
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ANISOU 1931  CG  PHE B  37     3979   4294   4111     -2     25     14       C
ATOM   1932  CD1 PHE B  37      10.725  28.128  48.253  1.00 31.78           C
ANISOU 1932  CD1 PHE B  37     3870   4151   4053     19     14     56       C
ATOM   1933  CD2 PHE B  37      11.752  28.680  46.171  1.00 32.67           C
ANISOU 1933  CD2 PHE B  37     4108   4218   4086    -24     24     65       C
ATOM   1934  CE1 PHE B  37      11.151  29.334  48.782  1.00 32.32           C
ANISOU 1934  CE1 PHE B  37     3985   4134   4160     36     -7     73       C
ATOM   1935  CE2 PHE B  37      12.187  29.874  46.702  1.00 32.84           C
ANISOU 1935  CE2 PHE B  37     4095   4228   4154    -11     45     46       C
ATOM   1936  CZ  PHE B  37      11.898  30.207  48.008  1.00 32.48           C
ANISOU 1936  CZ  PHE B  37     3993   4183   4165     33     37     68       C
ATOM   1937  N   LYS B  38       9.514  24.772  43.986  1.00 34.78           N
ANISOU 1937  N   LYS B  38     4435   4520   4258     -4     43     75       N
ATOM   1938  CA  LYS B  38       9.412  23.419  43.418  1.00 35.03           C
ANISOU 1938  CA  LYS B  38     4434   4480   4394     56     77     24       C
ATOM   1939  C   LYS B  38      10.835  23.151  42.930  1.00 35.27           C
ANISOU 1939  C   LYS B  38     4471   4531   4398     44     91     27       C
ATOM   1940  O   LYS B  38      11.370  23.978  42.186  1.00 35.51           O
ANISOU 1940  O   LYS B  38     4617   4626   4251    185    116    109       O
ATOM   1941  CB  LYS B  38       8.416  23.338  42.285  1.00 35.88           C
ANISOU 1941  CB  LYS B  38     4550   4670   4412     17     35     33       C
ATOM   1942  CG  LYS B  38       8.187  21.954  41.684  1.00 37.63           C
ANISOU 1942  CG  LYS B  38     4886   4732   4681    -13     59    -34       C
ATOM   1943  CD  LYS B  38       6.987  22.028  40.721  1.00 39.86           C
ANISOU 1943  CD  LYS B  38     5055   5177   4915    -37    -49    -21       C
ATOM   1944  CE  LYS B  38       6.566  20.634  40.272  1.00 40.85           C
ANISOU 1944  CE  LYS B  38     5294   5124   5104    -54    -17     44       C
ATOM   1945  NZ  LYS B  38       5.525  20.674  39.200  1.00 41.09           N
ANISOU 1945  NZ  LYS B  38     5071   5212   5330   -149     -8    -29       N
ATOM   1946  N   ILE B  39      11.508  22.203  43.548  1.00 35.56           N
ANISOU 1946  N   ILE B  39     4572   4566   4374     74    103     99       N
ATOM   1947  CA  ILE B  39      12.888  21.931  43.200  1.00 36.28           C
ANISOU 1947  CA  ILE B  39     4600   4666   4519     37    101     72       C
ATOM   1948  C   ILE B  39      13.052  20.418  43.021  1.00 37.20           C
ANISOU 1948  C   ILE B  39     4815   4709   4610     40     17     22       C
ATOM   1949  O   ILE B  39      12.144  19.633  43.269  1.00 37.22           O
ANISOU 1949  O   ILE B  39     5005   4663   4473     54    143     93       O
ATOM   1950  CB  ILE B  39      13.934  22.407  44.215  1.00 36.31           C
ANISOU 1950  CB  ILE B  39     4685   4600   4509     50     91     42       C
ATOM   1951  CG1 ILE B  39      13.690  21.786  45.602  1.00 35.97           C
ANISOU 1951  CG1 ILE B  39     4604   4581   4480     66     85     20       C
ATOM   1952  CG2 ILE B  39      13.984  23.926  44.280  1.00 36.35           C
ANISOU 1952  CG2 ILE B  39     4587   4609   4617     94     42     -2       C
ATOM   1953  CD1 ILE B  39      14.899  21.909  46.507  1.00 35.73           C
ANISOU 1953  CD1 ILE B  39     4679   4488   4410     78    103    -22       C
ATOM   1954  N   LYS B  40      14.224  20.092  42.497  1.00 38.39           N
ANISOU 1954  N   LYS B  40     4885   4980   4723     40     64     64       N
ATOM   1955  CA  LYS B  40      14.540  18.670  42.308  1.00 40.36           C
ANISOU 1955  CA  LYS B  40     5159   5087   5089     88      2    -12       C
ATOM   1956  C   LYS B  40      14.870  18.131  43.687  1.00 39.69           C
ANISOU 1956  C   LYS B  40     4975   5114   4991    100     91    -60       C
ATOM   1957  O   LYS B  40      15.482  18.878  44.467  1.00 39.08           O
ANISOU 1957  O   LYS B  40     4888   5122   4840    168    124    -20       O
ATOM   1958  CB  LYS B  40      15.692  18.623  41.310  1.00 42.50           C
ANISOU 1958  CB  LYS B  40     5274   5554   5320     36    107     36       C
ATOM   1959  CG  LYS B  40      15.963  17.289  40.673  1.00 45.10           C
ANISOU 1959  CG  LYS B  40     5778   5595   5762     41     21    -60       C
ATOM   1960  CD  LYS B  40      16.599  17.454  39.290  1.00 47.24           C
ANISOU 1960  CD  LYS B  40     6045   6017   5888    -11    120     38       C
ATOM   1961  CE  LYS B  40      16.925  16.080  38.717  1.00 48.47           C
ANISOU 1961  CE  LYS B  40     6184   6072   6161     32     75    -33       C
ATOM   1962  NZ  LYS B  40      17.025  16.097  37.230  1.00 49.86           N
ANISOU 1962  NZ  LYS B  40     6345   6392   6206     41     27     -3       N
ATOM   1963  N   ILE B  41      14.557  16.882  43.983  1.00 40.13           N
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ANISOU 1963  N   LYS B  41     5096   5144   5006    135    131    -35       N
ATOM   1964  CA  LYS B  41      14.899  16.318  45.286  1.00 40.89           C
ANISOU 1964  CA  LYS B  41     5280   5194   5062    102     45    -44       C
ATOM   1965  C   LYS B  41      16.389  16.230  45.541  1.00 40.76           C
ANISOU 1965  C   LYS B  41     5276   5133   5079    105     15    -35       C
ATOM   1966  O   LYS B  41      16.807  16.133  46.693  1.00 40.75           O
ANISOU 1966  O   LYS B  41     5350   5144   4991    235     82   -100       O
ATOM   1967  CB  LYS B  41      14.288  14.929  45.481  1.00 41.82           C
ANISOU 1967  CB  LYS B  41     5347   5259   5285     13     -6    -29       C
ATOM   1968  CG  LYS B  41      12.773  14.935  45.556  1.00 42.86           C
ANISOU 1968  CG  LYS B  41     5413   5418   5455     64     58    -38       C
ATOM   1969  CD  LYS B  41      12.231  13.519  45.685  1.00 43.64           C
ANISOU 1969  CD  LYS B  41     5585   5463   5533      9     25      5       C
ATOM   1970  CE  LYS B  41      10.715  13.496  45.785  1.00 44.40           C
ANISOU 1970  CE  LYS B  41     5621   5660   5588      7     23     23       C
ATOM   1971  NZ  LYS B  41      10.213  12.102  45.561  1.00 45.33           N
ANISOU 1971  NZ  LYS B  41     5790   5727   5707    -54     13      3       N
ATOM   1972  N   THR B  42      17.233  16.245  44.517  1.00 41.12           N
ANISOU 1972  N   THR B  42     5338   5248   5039    103     18     -9       N
ATOM   1973  CA  THR B  42      18.675  16.172  44.614  1.00 42.23           C
ANISOU 1973  CA  THR B  42     5363   5471   5211     96     53    -46       C
ATOM   1974  C   THR B  42      19.353  17.517  44.488  1.00 42.63           C
ANISOU 1974  C   THR B  42     5424   5538   5235     64     45     -9       C
ATOM   1975  O   THR B  42      20.585  17.660  44.487  1.00 42.26           O
ANISOU 1975  O   THR B  42     5409   5601   5047    127    170     25       O
ATOM   1976  CB  THR B  42      19.143  15.222  43.480  1.00 42.58           C
ANISOU 1976  CB  THR B  42     5404   5432   5342    104     47    -84       C
ATOM   1977  OG1 THR B  42      18.661  15.746  42.227  1.00 43.06           O
ANISOU 1977  OG1 THR B  42     5516   5531   5315    115     29   -113       O
ATOM   1978  CG2 THR B  42      18.582  13.827  43.689  1.00 42.38           C
ANISOU 1978  CG2 THR B  42     5284   5458   5362     81     37    -43       C
ATOM   1979  N   THR B  43      18.582  18.611  44.464  1.00 43.40           N
ANISOU 1979  N   THR B  43     5545   5622   5325    113     79     -5       N
ATOM   1980  CA  THR B  43      19.131  19.963  44.394  1.00 44.00           C
ANISOU 1980  CA  THR B  43     5568   5659   5491     54     63    -25       C
ATOM   1981  C   THR B  43      19.334  20.517  45.794  1.00 43.80           C
ANISOU 1981  C   THR B  43     5498   5638   5508     61     30     -3       C
ATOM   1982  O   THR B  43      18.456  20.385  46.642  1.00 43.49           O
ANISOU 1982  O   THR B  43     5646   5554   5325    129     49     53       O
ATOM   1983  CB  THR B  43      18.139  20.834  43.595  1.00 45.06           C
ANISOU 1983  CB  THR B  43     5689   5745   5686     38    -26     20       C
ATOM   1984  OG1 THR B  43      18.178  20.410  42.221  1.00 46.72           O
ANISOU 1984  OG1 THR B  43     6001   6030   5720     23     34    -18       O
ATOM   1985  CG2 THR B  43      18.425  22.317  43.673  1.00 44.21           C
ANISOU 1985  CG2 THR B  43     5508   5690   5601    102    -45     42       C
ATOM   1986  N   PRO B  44      20.487  21.096  46.087  1.00 44.05           N
ANISOU 1986  N   PRO B  44     5599   5639   5501     20      7    -14       N
ATOM   1987  CA  PRO B  44      20.749  21.675  47.387  1.00 42.79           C
ANISOU 1987  CA  PRO B  44     5415   5444   5397    114     63      6       C
ATOM   1988  C   PRO B  44      19.723  22.754  47.692  1.00 41.49           C
ANISOU 1988  C   PRO B  44     5222   5476   5068     64     74     39       C
ATOM   1989  O   PRO B  44      19.317  23.491  46.786  1.00 40.84           O
ANISOU 1989  O   PRO B  44     5169   5295   5052    121    222     40       O
ATOM   1990  CB  PRO B  44      22.131  22.311  47.261  1.00 43.55           C
ANISOU 1990  CB  PRO B  44     5485   5581   5480     12     22     37       C
ATOM   1991  CG  PRO B  44      22.775  21.623  46.095  1.00 44.15           C
ANISOU 1991  CG  PRO B  44     5555   5630   5589     41     37    -29       C
ATOM   1992  CD  PRO B  44      21.652  21.236  45.164  1.00 44.16           C
ANISOU 1992  CD  PRO B  44     5583   5673   5521     28     12      8       C
ATOM   1993  N   LEU B  45      19.382  22.927  48.968  1.00 39.39           N
ANISOU 1993  N   LEU B  45     4979   5050   4937    141     -4     11       N
ATOM   1994  CA  LEU B  45      18.420  23.958  49.355  1.00 37.24           C
ANISOU 1994  CA  LEU B  45     4669   4982   4497     12     44     69       C
ATOM   1995  C   LEU B  45      19.011  25.341  49.378  1.00 37.92           C
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ANISOU 1995  C   LEU B  45     4834   4960   4615     48     38     28       C
ATOM   1996  O   LEU B  45      18.296  26.333  49.591  1.00 37.54           O
ANISOU 1996  O   LEU B  45     4637   4940   4685     22     55    117       O
ATOM   1997  CB  LEU B  45      17.848  23.550  50.738  1.00 36.06           C
ANISOU 1997  CB  LEU B  45     4558   4675   4467     87     41      3       C
ATOM   1998  CG  LEU B  45      17.069  22.234  50.710  1.00 35.04           C
ANISOU 1998  CG  LEU B  45     4356   4630   4328    115     45      7       C
ATOM   1999  CD1 LEU B  45      16.969  21.611  52.105  1.00 35.04           C
ANISOU 1999  CD1 LEU B  45     4329   4589   4396    112      1     40       C
ATOM   2000  CD2 LEU B  45      15.652  22.438  50.176  1.00 35.12           C
ANISOU 2000  CD2 LEU B  45     4371   4602   4372     98     18     72       C
ATOM   2001  N   ARG B  46      20.324  25.505  49.161  1.00 38.69           N
ANISOU 2001  N   ARG B  46     4759   5158   4785    117     39     -5       N
ATOM   2002  CA  ARG B  46      20.959  26.808  49.231  1.00 40.79           C
ANISOU 2002  CA  ARG B  46     5198   5243   5058    -27     37     46       C
ATOM   2003  C   ARG B  46      20.201  27.889  48.481  1.00 40.42           C
ANISOU 2003  C   ARG B  46     4972   5268   5117    -57     67     60       C
ATOM   2004  O   ARG B  46      19.854  28.912  49.078  1.00 40.21           O
ANISOU 2004  O   ARG B  46     5052   5273   4953    -45    -38    113       O
ATOM   2005  CB  ARG B  46      22.413  26.739  48.744  1.00 43.60           C
ANISOU 2005  CB  ARG B  46     5272   5788   5504     94     33     25       C
ATOM   2006  CG  ARG B  46      23.143  28.074  48.696  1.00 47.01           C
ANISOU 2006  CG  ARG B  46     5940   5871   6050    -59    -84     38       C
ATOM   2007  CD  ARG B  46      24.446  27.936  47.919  1.00 50.57           C
ANISOU 2007  CD  ARG B  46     6281   6533   6399     66    146      0       C
ATOM   2008  NE  ARG B  46      25.391  29.034  48.116  1.00 53.51           N
ANISOU 2008  NE  ARG B  46     6766   6687   6879   -100     -6    -47       N
ATOM   2009  CZ  ARG B  46      26.694  28.973  47.808  1.00 55.02           C
ANISOU 2009  CZ  ARG B  46     6858   7009   7037    -16     60    -10       C
ATOM   2010  NH1 ARG B  46      27.223  27.861  47.288  1.00 55.70           N
ANISOU 2010  NH1 ARG B  46     7051   7039   7073     36     68     -9       N
ATOM   2011  NH2 ARG B  46      27.513  30.001  48.013  1.00 55.33           N
ANISOU 2011  NH2 ARG B  46     6921   7021   7079    -29     52    -25       N
ATOM   2012  N   ARG B  47      19.918  27.668  47.196  1.00 40.88           N
ANISOU 2012  N   ARG B  47     5065   5326   5141    -24     49     53       N
ATOM   2013  CA  ARG B  47      19.268  28.683  46.366  1.00 41.72           C
ANISOU 2013  CA  ARG B  47     5157   5397   5298     61      2     63       C
ATOM   2014  C   ARG B  47      17.910  29.080  46.925  1.00 40.16           C
ANISOU 2014  C   ARG B  47     5061   5228   4970    -33    -47     70       C
ATOM   2015  O   ARG B  47      17.553  30.253  47.068  1.00 40.12           O
ANISOU 2015  O   ARG B  47     4984   5230   5032    -53    -26    146       O
ATOM   2016  CB  ARG B  47      19.150  28.197  44.918  1.00 44.11           C
ANISOU 2016  CB  ARG B  47     5675   5648   5438    -10    -30    -33       C
ATOM   2017  CG  ARG B  47      20.485  28.035  44.191  1.00 46.48           C
ANISOU 2017  CG  ARG B  47     5763   6055   5843     24     48    -46       C
ATOM   2018  CD  ARG B  47      20.918  29.350  43.566  1.00 49.08           C
ANISOU 2018  CD  ARG B  47     6238   6175   6236    -46     95     60       C
ATOM   2019  NE  ARG B  47      20.086  29.649  42.391  1.00 51.08           N
ANISOU 2019  NE  ARG B  47     6421   6599   6386    -15    -45    -18       N
ATOM   2020  CZ  ARG B  47      20.035  30.869  41.858  1.00 52.78           C
ANISOU 2020  CZ  ARG B  47     6701   6658   6694    -20      6     38       C
ATOM   2021  NH1 ARG B  47      20.751  31.839  42.427  1.00 53.44           N
ANISOU 2021  NH1 ARG B  47     6795   6747   6764    -80     -8     -6       N
ATOM   2022  NH2 ARG B  47      19.288  31.158  40.793  1.00 53.59           N
ANISOU 2022  NH2 ARG B  47     6751   6903   6707    -38    -11     27       N
ATOM   2023  N   LEU B  48      17.163  28.069  47.338  1.00 39.03           N
ANISOU 2023  N   LEU B  48     4892   5095   4843     59    -62     -1       N
ATOM   2024  CA  LEU B  48      15.844  28.266  47.966  1.00 38.40           C
ANISOU 2024  CA  LEU B  48     4919   4986   4684      3    -39      4       C
ATOM   2025  C   LEU B  48      15.929  29.136  49.206  1.00 35.83           C
ANISOU 2025  C   LEU B  48     4434   4674   4505     72     25    129       C
ATOM   2026  O   LEU B  48      15.225  30.127  49.423  1.00 33.87           O
ANISOU 2026  O   LEU B  48     4272   4582   4015    -30    149    170       O
ATOM   2027  CB  LEU B  48      15.423  26.831  48.250  1.00 40.15           C
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ANISOU 2027  CB  LEU B  48     5145   5048   5061    -62    -38      7       C
ATOM   2028  CG  LEU B  48      14.111  26.471  48.907  1.00 40.86           C
ANISOU 2028  CG  LEU B  48     5187   5210   5127    -14     -3      7       C
ATOM   2029  CD1 LEU B  48      13.755  25.033  48.540  1.00 40.98           C
ANISOU 2029  CD1 LEU B  48     5215   5184   5173     -5    -20     18       C
ATOM   2030  CD2 LEU B  48      14.216  26.648  50.412  1.00 40.80           C
ANISOU 2030  CD2 LEU B  48     5218   5156   5129      2     -1     11       C
ATOM   2031  N   MET B  49      16.874  28.814  50.092  1.00 34.39           N
ANISOU 2031  N   MET B  49     4319   4518   4228      8    119     80       N
ATOM   2032  CA  MET B  49      17.116  29.539  51.333  1.00 34.12           C
ANISOU 2032  CA  MET B  49     4276   4389   4299     -3     51     69       C
ATOM   2033  C   MET B  49      17.583  30.969  51.101  1.00 34.71           C
ANISOU 2033  C   MET B  49     4408   4407   4372     -6    -55     88       C
ATOM   2034  O   MET B  49      17.141  31.906  51.768  1.00 35.24           O
ANISOU 2034  O   MET B  49     4471   4591   4326    -68    -36     10       O
ATOM   2035  CB  MET B  49      18.151  28.776  52.170  1.00 33.93           C
ANISOU 2035  CB  MET B  49     4280   4423   4188    -17     33     32       C
ATOM   2036  CG  MET B  49      17.684  27.370  52.538  1.00 34.25           C
ANISOU 2036  CG  MET B  49     4399   4404   4211      7     28     64       C
ATOM   2037  SD  MET B  49      19.052  26.281  53.024  1.00 34.57           S
ANISOU 2037  SD  MET B  49     4685   4519   3929    117    -48     74       S
ATOM   2038  CE  MET B  49      19.657  27.098  54.499  1.00 33.51           C
ANISOU 2038  CE  MET B  49     4492   4149   4091      7     -7     53       C
ATOM   2039  N   GLU B  50      18.483  31.134  50.133  1.00 35.37           N
ANISOU 2039  N   GLU B  50     4373   4612   4455     -5    -43     48       N
ATOM   2040  CA  GLU B  50      18.973  32.483  49.819  1.00 37.33           C
ANISOU 2040  CA  GLU B  50     4760   4685   4738    -32     39    142       C
ATOM   2041  C   GLU B  50      17.862  33.318  49.214  1.00 36.13           C
ANISOU 2041  C   GLU B  50     4613   4705   4408    -96    126    158       C
ATOM   2042  O   GLU B  50      17.652  34.472  49.616  1.00 36.27           O
ANISOU 2042  O   GLU B  50     4673   4633   4475    -69     30    282       O
ATOM   2043  CB  GLU B  50      20.220  32.371  48.938  1.00 40.63           C
ANISOU 2043  CB  GLU B  50     5035   5254   5147    -23    223     27       C
ATOM   2044  CG  GLU B  50      21.395  31.710  49.659  1.00 43.80           C
ANISOU 2044  CG  GLU B  50     5464   5582   5594     62   -106    117       C
ATOM   2045  CD  GLU B  50      22.628  31.649  48.780  1.00 46.59           C
ANISOU 2045  CD  GLU B  50     5800   6013   5887     62    103     17       C
ATOM   2046  OE1 GLU B  50      22.525  32.069  47.599  1.00 48.10           O
ANISOU 2046  OE1 GLU B  50     6083   6229   5963     98     32     65       O
ATOM   2047  OE2 GLU B  50      23.706  31.205  49.241  1.00 47.29           O
ANISOU 2047  OE2 GLU B  50     5930   6049   5988     96     -1     66       O
ATOM   2048  N   ALA B  51      17.014  32.728  48.391  1.00 36.59           N
ANISOU 2048  N   ALA B  51     4741   4700   4461    -48    100     92       N
ATOM   2049  CA  ALA B  51      15.878  33.424  47.783  1.00 36.88           C
ANISOU 2049  CA  ALA B  51     4770   4707   4537    -17     34     75       C
ATOM   2050  C   ALA B  51      14.925  33.921  48.856  1.00 37.40           C
ANISOU 2050  C   ALA B  51     4718   4807   4687      0     88    107       C
ATOM   2051  O   ALA B  51      14.507  35.084  48.874  1.00 37.53           O
ANISOU 2051  O   ALA B  51     4832   4823   4606    -26    115    218       O
ATOM   2052  CB  ALA B  51      15.153  32.517  46.806  1.00 37.13           C
ANISOU 2052  CB  ALA B  51     4688   4770   4650    -54      5     78       C
ATOM   2053  N   PHE B  52      14.601  33.017  49.800  1.00 37.58           N
ANISOU 2053  N   PHE B  52     4743   4831   4705     26     62    139       N
ATOM   2054  CA  PHE B  52      13.743  33.419  50.902  1.00 36.93           C
ANISOU 2054  CA  PHE B  52     4690   4678   4664     30     40    154       C
ATOM   2055  C   PHE B  52      14.340  34.569  51.694  1.00 37.67           C
ANISOU 2055  C   PHE B  52     4818   4750   4744    -48     48    146       C
ATOM   2056  O   PHE B  52      13.624  35.538  51.975  1.00 38.33           O
ANISOU 2056  O   PHE B  52     4861   4778   4924     11     13    161       O
ATOM   2057  CB  PHE B  52      13.465  32.237  51.841  1.00 35.85           C
ANISOU 2057  CB  PHE B  52     4469   4592   4561     -1     42      52       C
ATOM   2058  CG  PHE B  52      12.426  32.613  52.870  1.00 35.18           C
ANISOU 2058  CG  PHE B  52     4457   4478   4431    -25     -1     28       C
ATOM   2059  CD1 PHE B  52      11.084  32.470  52.572  1.00 35.08           C
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ANISOU 2059  CD1 PHE B  52     4447   4503   4380      7    -25     29       C
ATOM   2060  CD2 PHE B  52      12.780  33.118  54.107  1.00 34.44           C
ANISOU 2060  CD2 PHE B  52     4289   4369   4427    -32    -34     47       C
ATOM   2061  CE1 PHE B  52      10.112  32.806  53.487  1.00 34.97           C
ANISOU 2061  CE1 PHE B  52     4508   4384   4394     13      5     26       C
ATOM   2062  CE2 PHE B  52      11.797  33.479  55.018  1.00 34.48           C
ANISOU 2062  CE2 PHE B  52     4399   4372   4328    -28    -33     46       C
ATOM   2063  CZ  PHE B  52      10.467  33.323  54.709  1.00 34.37           C
ANISOU 2063  CZ  PHE B  52     4434   4265   4361    -14     -1     92       C
ATOM   2064  N   ALA B  53      15.604  34.495  52.090  1.00 38.42           N
ANISOU 2064  N   ALA B  53     4863   4808   4926     32     12    237       N
ATOM   2065  CA  ALA B  53      16.237  35.536  52.894  1.00 39.93           C
ANISOU 2065  CA  ALA B  53     5008   5046   5119    -34     19     72       C
ATOM   2066  C   ALA B  53      16.258  36.900  52.208  1.00 41.09           C
ANISOU 2066  C   ALA B  53     5200   5056   5356    -12     16     88       C
ATOM   2067  O   ALA B  53      15.906  37.943  52.769  1.00 40.06           O
ANISOU 2067  O   ALA B  53     5088   4979   5154   -216    149    133       O
ATOM   2068  CB  ALA B  53      17.677  35.102  53.193  1.00 40.13           C
ANISOU 2068  CB  ALA B  53     5088   5003   5155     11    -30    134       C
ATOM   2069  N   LYS B  54      16.643  36.878  50.936  1.00 43.57           N
ANISOU 2069  N   LYS B  54     5528   5564   5465    -12     77     36       N
ATOM   2070  CA  LYS B  54      16.728  38.069  50.089  1.00 45.45           C
ANISOU 2070  CA  LYS B  54     5911   5644   5712    -37     19     96       C
ATOM   2071  C   LYS B  54      15.370  38.753  50.048  1.00 47.50           C
ANISOU 2071  C   LYS B  54     6043   6021   5983     98     25     77       C
ATOM   2072  O   LYS B  54      15.272  39.951  50.325  1.00 47.24           O
ANISOU 2072  O   LYS B  54     5943   6011   5997     33      6     76       O
ATOM   2073  CB  LYS B  54      17.191  37.688  48.700  1.00 45.58           C
ANISOU 2073  CB  LYS B  54     5829   5754   5737    -27     43     75       C
ATOM   2074  N   ARG B  55      14.302  37.984  49.836  1.00 49.68           N
ANISOU 2074  N   ARG B  55     6363   6251   6261    -87    -40     45       N
ATOM   2075  CA  ARG B  55      12.965  38.572  49.877  1.00 51.93           C
ANISOU 2075  CA  ARG B  55     6546   6594   6589     90     13     57       C
ATOM   2076  C   ARG B  55      12.618  39.243  51.196  1.00 52.04           C
ANISOU 2076  C   ARG B  55     6571   6574   6625     10     30     23       C
ATOM   2077  O   ARG B  55      11.855  40.222  51.179  1.00 51.46           O
ANISOU 2077  O   ARG B  55     6615   6515   6424      1    -10     63       O
ATOM   2078  CB  ARG B  55      11.887  37.564  49.499  1.00 54.25           C
ANISOU 2078  CB  ARG B  55     6811   6778   7022    -70     25     11       C
ATOM   2079  CG  ARG B  55      11.502  37.719  48.028  1.00 57.16           C
ANISOU 2079  CG  ARG B  55     7336   7253   7127    -23    -30     20       C
ATOM   2080  CD  ARG B  55       9.984  37.592  47.893  1.00 59.38           C
ANISOU 2080  CD  ARG B  55     7398   7582   7583     -3     -5     61       C
ATOM   2081  NE  ARG B  55       9.710  36.806  46.692  1.00 61.03           N
ANISOU 2081  NE  ARG B  55     7771   7742   7674     12    -24    -10       N
ATOM   2082  CZ  ARG B  55       8.543  36.267  46.382  1.00 62.13           C
ANISOU 2082  CZ  ARG B  55     7830   7885   7892    -34    -52     26       C
ATOM   2083  NH1 ARG B  55       7.503  36.433  47.191  1.00 62.74           N
ANISOU 2083  NH1 ARG B  55     7936   7955   7948     24     -5     19       N
ATOM   2084  NH2 ARG B  55       8.461  35.570  45.256  1.00 62.58           N
ANISOU 2084  NH2 ARG B  55     7907   7940   7929    -12      2    -10       N
ATOM   2085  N   GLN B  56      13.149  38.796  52.333  1.00 52.31           N
ANISOU 2085  N   GLN B  56     6603   6578   6693     46      0     58       N
ATOM   2086  CA  GLN B  56      12.893  39.457  53.600  1.00 53.36           C
ANISOU 2086  CA  GLN B  56     6781   6761   6734     53    -13     16       C
ATOM   2087  C   GLN B  56      13.927  40.547  53.850  1.00 53.81           C
ANISOU 2087  C   GLN B  56     6817   6773   6855     47    -41     44       C
ATOM   2088  O   GLN B  56      13.934  41.194  54.894  1.00 54.10           O
ANISOU 2088  O   GLN B  56     6871   6810   6874     33    -32     32       O
ATOM   2089  CB  GLN B  56      12.924  38.482  54.781  1.00 53.69           C
ANISOU 2089  CB  GLN B  56     6799   6802   6799     44     -3     50       C
ATOM   2090  CG  GLN B  56      12.304  37.127  54.536  1.00 54.05           C
ANISOU 2090  CG  GLN B  56     6863   6836   6838     -1     21     23       C
ATOM   2091  CD  GLN B  56      10.941  37.214  53.878  1.00 54.55           C
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ANISOU 2091  CD  GLN B  56     6915   6923   6888      5     -8     24       C
ATOM   2092  OE1 GLN B  56      10.150  38.109  54.195  1.00 55.10           O
ANISOU 2092  OE1 GLN B  56     6998   6968   6969     38      4      1       O
ATOM   2093  NE2 GLN B  56      10.690  36.309  52.944  1.00 54.32           N
ANISOU 2093  NE2 GLN B  56     6879   6860   6901      5      6     28       N
ATOM   2094  N   GLY B  57      14.899  40.680  52.958  1.00 54.34           N
ANISOU 2094  N   GLY B  57     6876   6886   6885     69    -26     51       N
ATOM   2095  CA  GLY B  57      15.988  41.638  53.073  1.00 55.13           C
ANISOU 2095  CA  GLY B  57     6995   6945   7008     -2     -5     16       C
ATOM   2096  C   GLY B  57      16.907  41.276  54.241  1.00 55.51           C
ANISOU 2096  C   GLY B  57     7060   7008   7025     14    -22     39       C
ATOM   2097  O   GLY B  57      17.584  42.131  54.812  1.00 56.13           O
ANISOU 2097  O   GLY B  57     7178   7006   7144    -24     -9     40       O
ATOM   2098  N   LYS B  58      16.933  39.999  54.615  1.00 55.18           N
ANISOU 2098  N   LYS B  58     7016   6970   6980     27    -38      3       N
ATOM   2099  CA  LYS B  58      17.696  39.522  55.748  1.00 54.66           C
ANISOU 2099  CA  LYS B  58     6942   6883   6941     16    -10    -22       C
ATOM   2100  C   LYS B  58      18.916  38.715  55.326  1.00 53.98           C
ANISOU 2100  C   LYS B  58     6864   6793   6851    -26    -23     41       C
ATOM   2101  O   LYS B  58      18.947  38.065  54.287  1.00 53.68           O
ANISOU 2101  O   LYS B  58     6841   6721   6833    -11    -11     67       O
ATOM   2102  CB  LYS B  58      16.824  38.670  56.683  1.00 55.17           C
ANISOU 2102  CB  LYS B  58     6977   7015   6972    -15    -29     45       C
ATOM   2103  CG  LYS B  58      15.946  39.522  57.589  1.00 56.18           C
ANISOU 2103  CG  LYS B  58     7104   7131   7110     30      9     -5       C
ATOM   2104  CD  LYS B  58      14.899  38.691  58.321  1.00 56.75           C
ANISOU 2104  CD  LYS B  58     7176   7201   7188    -20     18     14       C
ATOM   2105  CE  LYS B  58      13.769  39.572  58.836  1.00 56.84           C
ANISOU 2105  CE  LYS B  58     7180   7227   7190     -2     -2      4       C
ATOM   2106  NZ  LYS B  58      12.753  38.784  59.589  1.00 56.81           N
ANISOU 2106  NZ  LYS B  58     7186   7209   7191    -18    -19     -2       N
ATOM   2107  N   GLU B  59      19.912  38.785  56.202  1.00 53.55           N
ANISOU 2107  N   GLU B  59     6802   6702   6841      3     12     26       N
ATOM   2108  CA  GLU B  59      21.151  38.052  55.964  1.00 53.20           C
ANISOU 2108  CA  GLU B  59     6759   6698   6756    -25      1     31       C
ATOM   2109  C   GLU B  59      20.927  36.584  56.321  1.00 52.61           C
ANISOU 2109  C   GLU B  59     6645   6654   6691     -3     -5     -6       C
ATOM   2110  O   GLU B  59      20.245  36.249  57.290  1.00 52.52           O
ANISOU 2110  O   GLU B  59     6593   6603   6758    -72    -14     -7       O
ATOM   2111  CB  GLU B  59      22.275  38.670  56.777  1.00 53.05           C
ANISOU 2111  CB  GLU B  59     6720   6688   6749      7     16      6       C
ATOM   2112  N   MET B  60      21.545  35.709  55.554  1.00 51.89           N
ANISOU 2112  N   MET B  60     6548   6588   6579    -25    -23     35       N
ATOM   2113  CA  MET B  60      21.509  34.279  55.744  1.00 51.70           C
ANISOU 2113  CA  MET B  60     6527   6576   6539    -31     13    -12       C
ATOM   2114  C   MET B  60      22.019  33.785  57.084  1.00 52.12           C
ANISOU 2114  C   MET B  60     6605   6602   6595    -25    -14     22       C
ATOM   2115  O   MET B  60      21.512  32.787  57.592  1.00 52.65           O
ANISOU 2115  O   MET B  60     6718   6658   6629    -47     65     38       O
ATOM   2116  CB  MET B  60      22.430  33.652  54.674  1.00 50.92           C
ANISOU 2116  CB  MET B  60     6441   6458   6448    -53    -52    -12       C
ATOM   2117  CG  MET B  60      21.681  33.554  53.340  1.00 49.61           C
ANISOU 2117  CG  MET B  60     6237   6262   6349   -104     32     22       C
ATOM   2118  SD  MET B  60      20.383  32.315  53.571  1.00 47.67           S
ANISOU 2118  SD  MET B  60     6200   6065   5846    -53     88     25       S
ATOM   2119  CE  MET B  60      21.295  30.826  53.148  1.00 47.57           C
ANISOU 2119  CE  MET B  60     5978   6078   6017    -47     -1     38       C
ATOM   2120  N   ASP B  61      23.008  34.447  57.670  1.00 51.70           N
ANISOU 2120  N   ASP B  61     6571   6566   6506      3    -16     42       N
ATOM   2121  CA  ASP B  61      23.620  34.033  58.924  1.00 51.25           C
ANISOU 2121  CA  ASP B  61     6528   6495   6450     39     41     -6       C
ATOM   2122  C   ASP B  61      22.831  34.462  60.151  1.00 49.03           C
ANISOU 2122  C   ASP B  61     6135   6161   6334      4    -53     87       C
ATOM   2123  O   ASP B  61      23.231  34.204  61.290  1.00 49.30           O
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ANISOU 2123  O   ASP B  61     6278   6190   6265    -37     -4     52       O
ATOM   2124  CB  ASP B  61      25.069  34.545  58.999  1.00 53.17           C
ANISOU 2124  CB  ASP B  61     6602   6824   6775    -24    -17     31       C
ATOM   2125  CG  ASP B  61      25.258  36.036  59.112  1.00 54.52           C
ANISOU 2125  CG  ASP B  61     6875   6880   6959    -36     -7     14       C
ATOM   2126  OD1 ASP B  61      24.273  36.810  59.043  1.00 55.35           O
ANISOU 2126  OD1 ASP B  61     6932   6971   7126      7    -25     47       O
ATOM   2127  OD2 ASP B  61      26.412  36.510  59.285  1.00 55.04           O
ANISOU 2127  OD2 ASP B  61     6826   7093   6996    -10      4     64       O
ATOM   2128  N   SER B  62      21.732  35.163  59.923  1.00 46.10           N
ANISOU 2128  N   SER B  62     5834   5852   5830   -146    113     15       N
ATOM   2129  CA  SER B  62      20.838  35.649  60.948  1.00 43.53           C
ANISOU 2129  CA  SER B  62     5380   5499   5660   -192    -71     67       C
ATOM   2130  C   SER B  62      19.565  34.787  60.955  1.00 39.77           C
ANISOU 2130  C   SER B  62     5122   4983   5004     38    -49     50       C
ATOM   2131  O   SER B  62      18.728  35.038  61.816  1.00 38.68           O
ANISOU 2131  O   SER B  62     4909   4953   4834    -66   -104    243       O
ATOM   2132  CB  SER B  62      20.446  37.109  60.705  1.00 45.00           C
ANISOU 2132  CB  SER B  62     5683   5603   5811    -42      3     59       C
ATOM   2133  OG  SER B  62      19.630  37.220  59.536  1.00 47.01           O
ANISOU 2133  OG  SER B  62     6007   5955   5900    -19   -100     81       O
ATOM   2134  N   LEU B  63      19.450  33.905  59.967  1.00 36.26           N
ANISOU 2134  N   LEU B  63     4488   4427   4862    -86    -40    304       N
ATOM   2135  CA  LEU B  63      18.258  33.067  59.870  1.00 33.71           C
ANISOU 2135  CA  LEU B  63     4289   4044   4475     62     18    165       C
ATOM   2136  C   LEU B  63      18.609  31.578  59.971  1.00 31.59           C
ANISOU 2136  C   LEU B  63     3950   3949   4104    -55     90    280       C
ATOM   2137  O   LEU B  63      19.568  31.099  59.371  1.00 31.78           O
ANISOU 2137  O   LEU B  63     4105   3811   4158     22    160    417       O
ATOM   2138  CB  LEU B  63      17.522  33.173  58.529  1.00 34.61           C
ANISOU 2138  CB  LEU B  63     4385   4316   4448     26     33     98       C
ATOM   2139  CG  LEU B  63      16.682  34.423  58.257  1.00 35.54           C
ANISOU 2139  CG  LEU B  63     4540   4433   4530    127    -34     78       C
ATOM   2140  CD1 LEU B  63      16.227  34.429  56.803  1.00 35.42           C
ANISOU 2140  CD1 LEU B  63     4525   4436   4498     70    -11     53       C
ATOM   2141  CD2 LEU B  63      15.482  34.503  59.180  1.00 35.92           C
ANISOU 2141  CD2 LEU B  63     4568   4534   4546     14    -12    126       C
ATOM   2142  N   ARG B  64      17.816  30.831  60.730  1.00 28.52           N
ANISOU 2142  N   ARG B  64     3433   3671   3733    -28    -93     74       N
ATOM   2143  CA  ARG B  64      18.010  29.398  60.822  1.00 25.81           C
ANISOU 2143  CA  ARG B  64     3105   3587   3114     19    -14     56       C
ATOM   2144  C   ARG B  64      16.848  28.717  60.090  1.00 26.11           C
ANISOU 2144  C   ARG B  64     3216   3542   3163     33     -1    -39       C
ATOM   2145  O   ARG B  64      15.688  29.012  60.406  1.00 27.40           O
ANISOU 2145  O   ARG B  64     3283   3730   3399     19    -51   -117       O
ATOM   2146  CB  ARG B  64      17.989  28.920  62.295  1.00 26.53           C
ANISOU 2146  CB  ARG B  64     3394   3612   3073    -34     23      60       C
ATOM   2147  CG  ARG B  64      18.821  29.807  63.229  1.00 26.50           C
ANISOU 2147  CG  ARG B  64     3533   3550   2984    -32      2    113       C
ATOM   2148  CD  ARG B  64      20.293  29.729  62.903  1.00 27.50           C
ANISOU 2148  CD  ARG B  64     3535   3681   3234   -126    -63    134       C
ATOM   2149  NE  ARG B  64      21.105  30.383  63.937  1.00 27.46           N
ANISOU 2149  NE  ARG B  64     3606   3654   3173    -64   -109    200       N
ATOM   2150  CZ  ARG B  64      21.834  31.451  63.767  1.00 27.33           C
ANISOU 2150  CZ  ARG B  64     3492   3567   3325    -93   -116     60       C
ATOM   2151  NH1 ARG B  64      21.926  32.034  62.561  1.00 29.19           N
ANISOU 2151  NH1 ARG B  64     3723   3917   3453   -188     17    196       N
ATOM   2152  NH2 ARG B  64      22.509  31.932  64.798  1.00 26.04           N
ANISOU 2152  NH2 ARG B  64     3462   3343   3088     73    -45    219       N
ATOM   2153  N   PHE B  65      17.150  27.845  59.156  1.00 24.96           N
ANISOU 2153  N   PHE B  65     3251   3243   2990     14    -85     64       N
ATOM   2154  CA  PHE B  65      16.116  27.166  58.385  1.00 25.66           C
ANISOU 2154  CA  PHE B  65     3183   3370   3197    -48      1     93       C
ATOM   2155  C   PHE B  65      15.971  25.753  58.935  1.00 25.10           C
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ANISOU 2155  C   PHE B  65     3260   3368   2909     -7     -5     87       C
ATOM   2156  O   PHE B  65      16.918  24.959  58.899  1.00 25.00           O
ANISOU 2156  O   PHE B  65     3165   3822   2513     70    148    188       O
ATOM   2157  CB  PHE B  65      16.467  27.129  56.892  1.00 27.19           C
ANISOU 2157  CB  PHE B  65     3405   3704   3222     30     21     -8       C
ATOM   2158  CG  PHE B  65      16.501  28.473  56.236  1.00 29.68           C
ANISOU 2158  CG  PHE B  65     3870   3847   3558      2      8     92       C
ATOM   2159  CD1 PHE B  65      17.643  29.247  56.227  1.00 30.70           C
ANISOU 2159  CD1 PHE B  65     3780   3994   3889    -17    -18      3       C
ATOM   2160  CD2 PHE B  65      15.366  28.933  55.565  1.00 30.32           C
ANISOU 2160  CD2 PHE B  65     3722   3977   3823     50     50     55       C
ATOM   2161  CE1 PHE B  65      17.645  30.478  55.601  1.00 31.72           C
ANISOU 2161  CE1 PHE B  65     3904   4119   4030    -64     34    119       C
ATOM   2162  CE2 PHE B  65      15.369  30.171  54.941  1.00 31.21           C
ANISOU 2162  CE2 PHE B  65     3981   4020   3859    -30    -13     63       C
ATOM   2163  CZ  PHE B  65      16.518  30.945  54.947  1.00 31.82           C
ANISOU 2163  CZ  PHE B  65     4038   4097   3956    -43    -27     62       C
ATOM   2164  N   LEU B  66      14.805  25.470  59.517  1.00 24.98           N
ANISOU 2164  N   LEU B  66     3149   3442   2899     96    -32     17       N
ATOM   2165  CA  LEU B  66      14.597  24.165  60.144  1.00 25.89           C
ANISOU 2165  CA  LEU B  66     3215   3385   3239    -43   -104    -26       C
ATOM   2166  C   LEU B  66      13.529  23.314  59.446  1.00 26.86           C
ANISOU 2166  C   LEU B  66     3401   3441   3366     11    -94    -46       C
ATOM   2167  O   LEU B  66      12.525  23.841  58.991  1.00 25.08           O
ANISOU 2167  O   LEU B  66     3185   3287   3056    168     90     32       O
ATOM   2168  CB  LEU B  66      14.094  24.367  61.583  1.00 27.45           C
ANISOU 2168  CB  LEU B  66     3450   3620   3359    -57     33     12       C
ATOM   2169  CG  LEU B  66      14.853  25.302  62.513  1.00 28.71           C
ANISOU 2169  CG  LEU B  66     3449   3948   3512    -73    -71    -65       C
ATOM   2170  CD1 LEU B  66      14.350  25.151  63.959  1.00 29.40           C
ANISOU 2170  CD1 LEU B  66     3581   3947   3641   -168    134   -118       C
ATOM   2171  CD2 LEU B  66      16.353  25.078  62.517  1.00 28.52           C
ANISOU 2171  CD2 LEU B  66     3518   3884   3435     90    -10     -5       C
ATOM   2172  N   TYR B  67      13.776  22.012  59.487  1.00 26.50           N
ANISOU 2172  N   TYR B  67     3492   3391   3184    -11     32    -14       N
ATOM   2173  CA  TYR B  67      12.813  21.076  58.923  1.00 27.08           C
ANISOU 2173  CA  TYR B  67     3458   3523   3306    -66      6    -29       C
ATOM   2174  C   TYR B  67      12.511  20.057  60.012  1.00 25.68           C
ANISOU 2174  C   TYR B  67     3271   3392   3096    -78    -94   -146       C
ATOM   2175  O   TYR B  67      13.345  19.256  60.402  1.00 24.58           O
ANISOU 2175  O   TYR B  67     3156   3434   2748    -63     55   -352       O
ATOM   2176  CB  TYR B  67      13.360  20.413  57.648  1.00 28.18           C
ANISOU 2176  CB  TYR B  67     3622   3669   3416     30     83    -76       C
ATOM   2177  CG  TYR B  67      12.490  19.221  57.259  1.00 28.18           C
ANISOU 2177  CG  TYR B  67     3741   3612   3353     12    110    -29       C
ATOM   2178  CD1 TYR B  67      11.175  19.433  56.866  1.00 28.95           C
ANISOU 2178  CD1 TYR B  67     3756   3712   3532    -84     35    -42       C
ATOM   2179  CD2 TYR B  67      12.989  17.925  57.312  1.00 27.79           C
ANISOU 2179  CD2 TYR B  67     3770   3595   3195      3     78     49       C
ATOM   2180  CE1 TYR B  67      10.352  18.367  56.521  1.00 29.96           C
ANISOU 2180  CE1 TYR B  67     4031   3710   3643    -82    -40    -93       C
ATOM   2181  CE2 TYR B  67      12.179  16.855  56.979  1.00 29.12           C
ANISOU 2181  CE2 TYR B  67     3882   3755   3428    -85     41     11       C
ATOM   2182  CZ  TYR B  67      10.879  17.091  56.599  1.00 29.69           C
ANISOU 2182  CZ  TYR B  67     3880   3765   3635    -19    -29     15       C
ATOM   2183  OH  TYR B  67      10.053  16.050  56.259  1.00 32.14           O
ANISOU 2183  OH  TYR B  67     4228   3907   4076   -207   -125    -40       O
ATOM   2184  N   ASP B  68      11.328  20.184  60.624  1.00 25.56           N
ANISOU 2184  N   ASP B  68     3323   3377   3013    -64    -85   -220       N
ATOM   2185  CA  ASP B  68      10.923  19.276  61.701  1.00 27.04           C
ANISOU 2185  CA  ASP B  68     3416   3539   3318    -89   -189     -6       C
ATOM   2186  C   ASP B  68      11.935  19.318  62.854  1.00 25.55           C
ANISOU 2186  C   ASP B  68     3276   3275   3155    -13    -99     12       C
ATOM   2187  O   ASP B  68      12.308  18.287  63.430  1.00 24.29           O
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ANISOU 2187  O   ASP B  68     2889   3283   3057    -89   -100     81       O
ATOM   2188  CB  ASP B  68      10.787  17.846  61.173  1.00 29.17           C
ANISOU 2188  CB  ASP B  68     3729   3609   3746      2   -118   -136       C
ATOM   2189  CG  ASP B  68       9.492  17.622  60.395  1.00 31.97           C
ANISOU 2189  CG  ASP B  68     3862   4198   4086    -31   -185    -96       C
ATOM   2190  OD1 ASP B  68       8.669  18.547  60.309  1.00 31.80           O
ANISOU 2190  OD1 ASP B  68     4010   4054   4019    -47   -294    -70       O
ATOM   2191  OD2 ASP B  68       9.343  16.483  59.886  1.00 33.94           O
ANISOU 2191  OD2 ASP B  68     4243   4375   4279   -212   -207   -225       O
ATOM   2192  N   GLY B  69      12.460  20.510  63.090  1.00 24.44           N
ANISOU 2192  N   GLY B  69     3073   3243   2968    -80   -149     62       N
ATOM   2193  CA  GLY B  69      13.428  20.760  64.143  1.00 23.71           C
ANISOU 2193  CA  GLY B  69     3004   3167   2839    112    -78    -53       C
ATOM   2194  C   GLY B  69      14.873  20.590  63.761  1.00 23.88           C
ANISOU 2194  C   GLY B  69     2884   3229   2962   -103   -124   -147       C
ATOM   2195  O   GLY B  69      15.755  20.896  64.594  1.00 24.06           O
ANISOU 2195  O   GLY B  69     2885   3344   2914    186   -167   -406       O
ATOM   2196  N   ILE B  70      15.170  20.055  62.592  1.00 23.99           N
ANISOU 2196  N   ILE B  70     2900   3280   2936    -39    -44   -185       N
ATOM   2197  CA  ILE B  70      16.563  19.855  62.146  1.00 25.40           C
ANISOU 2197  CA  ILE B  70     3104   3353   3194    -34      8   -114       C
ATOM   2198  C   ILE B  70      17.077  21.096  61.443  1.00 25.08           C
ANISOU 2198  C   ILE B  70     2947   3416   3167    -13    -60      2       C
ATOM   2199  O   ILE B  70      16.453  21.601  60.493  1.00 24.99           O
ANISOU 2199  O   ILE B  70     2896   3652   2949   -181   -243   -174       O
ATOM   2200  CB  ILE B  70      16.623  18.674  61.143  1.00 26.14           C
ANISOU 2200  CB  ILE B  70     3251   3398   3282     58    108   -158       C
ATOM   2201  CG1 ILE B  70      16.156  17.377  61.801  1.00 27.39           C
ANISOU 2201  CG1 ILE B  70     3550   3439   3417     39     14   -133       C
ATOM   2202  CG2 ILE B  70      18.054  18.550  60.587  1.00 25.18           C
ANISOU 2202  CG2 ILE B  70     3176   3286   3105    180    -12   -222       C
ATOM   2203  CD1 ILE B  70      15.876  16.352  60.695  1.00 28.46           C
ANISOU 2203  CD1 ILE B  70     3730   3619   3462      7      7   -215       C
ATOM   2204  N   ARG B  71      18.229  21.606  61.881  1.00 23.27           N
ANISOU 2204  N   ARG B  71     2979   2921   2943     12    -39   -168       N
ATOM   2205  CA  ARG B  71      18.819  22.806  61.317  1.00 25.13           C
ANISOU 2205  CA  ARG B  71     3253   3205   3091    -57    -37    -42       C
ATOM   2206  C   ARG B  71      19.495  22.455  59.998  1.00 26.72           C
ANISOU 2206  C   ARG B  71     3226   3613   3314    -28    150      8       C
ATOM   2207  O   ARG B  71      20.522  21.782  59.974  1.00 27.96           O
ANISOU 2207  O   ARG B  71     3497   3836   3291    231    -78    -32       O
ATOM   2208  CB  ARG B  71      19.868  23.329  62.302  1.00 24.76           C
ANISOU 2208  CB  ARG B  71     3195   3105   3109    -10    -99       2       C
ATOM   2209  CG  ARG B  71      20.440  24.691  61.899  1.00 25.29           C
ANISOU 2209  CG  ARG B  71     3258   3194   3159    -82     44    -72       C
ATOM   2210  CD  ARG B  71      21.710  24.989  62.720  1.00 26.18           C
ANISOU 2210  CD  ARG B  71     3244   3466   3238    -64    -10    -74       C
ATOM   2211  NE  ARG B  71      21.245  25.193  64.120  1.00 26.72           N
ANISOU 2211  NE  ARG B  71     3435   3475   3244     80     -3   -111       N
ATOM   2212  CZ  ARG B  71      21.488  26.324  64.774  1.00 26.12           C
ANISOU 2212  CZ  ARG B  71     3232   3521   3173     32     -2    -72       C
ATOM   2213  NH1 ARG B  71      22.159  27.310  64.198  1.00 27.62           N
ANISOU 2213  NH1 ARG B  71     3751   3409   3336    -10    -90     20       N
ATOM   2214  NH2 ARG B  71      21.009  26.447  66.019  1.00 24.03           N
ANISOU 2214  NH2 ARG B  71     3088   3164   2879    212   -289    -99       N
ATOM   2215  N   ILE B  72      18.888  22.889  58.917  1.00 27.53           N
ANISOU 2215  N   ILE B  72     3315   3727   3418      6     71      57       N
ATOM   2216  CA  ILE B  72      19.378  22.637  57.571  1.00 28.63           C
ANISOU 2216  CA  ILE B  72     3465   3869   3542     84     92      -7       C
ATOM   2217  C   ILE B  72      20.679  23.392  57.304  1.00 30.30           C
ANISOU 2217  C   ILE B  72     3693   3999   3819    -34     73      45       C
ATOM   2218  O   ILE B  72      20.893  24.548  57.640  1.00 29.09           O
ANISOU 2218  O   ILE B  72     3254   3987   3811     24   185      70       O
ATOM   2219  CB  ILE B  72      18.333  23.078  56.537  1.00 29.16           C
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ANISOU 2219  CB  ILE B  72     3555   3934   3592    -32     10     44       C
ATOM   2220  CG1 ILE B  72      17.010  22.329  56.770  1.00 28.08           C
ANISOU 2220  CG1 ILE B  72     3377   3804   3489     20    -65     29       C
ATOM   2221  CG2 ILE B  72      18.784  22.783  55.120  1.00 29.87           C
ANISOU 2221  CG2 ILE B  72     3734   4025   3590    121     -2      6       C
ATOM   2222  CD1 ILE B  72      15.864  23.035  56.009  1.00 27.23           C
ANISOU 2222  CD1 ILE B  72     3428   3606   3314     22    -74     35       C
ATOM   2223  N   GLN B  73      21.553  22.631  56.658  1.00 32.41           N
ANISOU 2223  N   GLN B  73     3967   4343   4005    225     82     46       N
ATOM   2224  CA  GLN B  73      22.830  23.207  56.198  1.00 35.61           C
ANISOU 2224  CA  GLN B  73     4338   4637   4556   -118    143     98       C
ATOM   2225  C   GLN B  73      22.603  23.430  54.694  1.00 37.25           C
ANISOU 2225  C   GLN B  73     4631   4894   4628      0      2     29       C
ATOM   2226  O   GLN B  73      22.109  22.545  53.991  1.00 36.37           O
ANISOU 2226  O   GLN B  73     4495   4824   4500    -11    144     56       O
ATOM   2227  CB  GLN B  73      23.977  22.265  56.532  1.00 37.02           C
ANISOU 2227  CB  GLN B  73     4602   4820   4645     71     59     36       C
ATOM   2228  CG  GLN B  73      25.375  22.878  56.447  1.00 38.88           C
ANISOU 2228  CG  GLN B  73     4790   5080   4901    -61     33    -20       C
ATOM   2229  CD  GLN B  73      25.906  22.962  55.028  1.00 39.95           C
ANISOU 2229  CD  GLN B  73     5035   5183   4960     -9     63      6       C
ATOM   2230  OE1 GLN B  73      25.656  22.086  54.197  1.00 40.10           O
ANISOU 2230  OE1 GLN B  73     5044   5390   4803    -70     19    -15       O
ATOM   2231  NE2 GLN B  73      26.645  24.024  54.736  1.00 40.37           N
ANISOU 2231  NE2 GLN B  73     5030   5299   5011    -66     62     43       N
ATOM   2232  N   ALA B  74      22.920  24.646  54.235  1.00 39.00           N
ANISOU 2232  N   ALA B  74     4856   4933   5027    -14     76     81       N
ATOM   2233  CA  ALA B  74      22.697  24.979  52.817  1.00 41.23           C
ANISOU 2233  CA  ALA B  74     5221   5314   5130    -36    -33     86       C
ATOM   2234  C   ALA B  74      23.427  23.938  52.003  1.00 42.80           C
ANISOU 2234  C   ALA B  74     5445   5453   5364    -52     95    -26       C
ATOM   2235  O   ALA B  74      24.478  23.548  52.524  1.00 44.84           O
ANISOU 2235  O   ALA B  74     5616   5781   5640     86     77     32       O
ATOM   2236  CB  ALA B  74      23.220  26.371  52.507  1.00 41.18           C
ANISOU 2236  CB  ALA B  74     5213   5260   5175    -30    -10      2       C
ATOM   2237  N   ASP B  75      22.984  23.374  50.882  1.00 43.38           N
ANISOU 2237  N   ASP B  75     5569   5523   5393    -47    117    -63       N
ATOM   2238  CA  ASP B  75      23.920  22.331  50.362  1.00 42.67           C
ANISOU 2238  CA  ASP B  75     5413   5411   5387    -48     64     26       C
ATOM   2239  C   ASP B  75      23.413  20.947  50.702  1.00 40.94           C
ANISOU 2239  C   ASP B  75     5140   5349   5066     20    121     18       C
ATOM   2240  O   ASP B  75      23.780  19.968  50.046  1.00 41.04           O
ANISOU 2240  O   ASP B  75     5068   5417   5109     74     92    -28       O
ATOM   2241  N   GLN B  76      22.576  20.843  51.735  1.00 39.10           N
ANISOU 2241  N   GLN B  76     4907   4999   4949     51     47      -5       N
ATOM   2242  CA  GLN B  76      21.884  19.598  52.000  1.00 36.70           C
ANISOU 2242  CA  GLN B  76     4653   4850   4442    122     23    -44       C
ATOM   2243  C   GLN B  76      20.705  19.672  50.993  1.00 35.71           C
ANISOU 2243  C   GLN B  76     4500   4682   4386     58    117    -28       C
ATOM   2244  O   GLN B  76      20.273  20.782  50.645  1.00 35.70           O
ANISOU 2244  O   GLN B  76     4506   4670   4389     73    157    -26       O
ATOM   2245  CB  GLN B  76      21.275  19.429  53.390  1.00 36.16           C
ANISOU 2245  CB  GLN B  76     4548   4751   4439     72     19    -11       C
ATOM   2246  CG  GLN B  76      22.308  19.265  54.507  1.00 35.85           C
ANISOU 2246  CG  GLN B  76     4452   4742   4428     93     68      9       C
ATOM   2247  CD  GLN B  76      21.613  18.955  55.829  1.00 35.73           C
ANISOU 2247  CD  GLN B  76     4666   4592   4316     66    -48     21       C
ATOM   2248  OE1 GLN B  76      21.081  19.855  56.481  1.00 34.71           O
ANISOU 2248  OE1 GLN B  76     4189   4657   4344    147     14     78       O
ATOM   2249  NE2 GLN B  76      21.633  17.669  56.182  1.00 35.30           N
ANISOU 2249  NE2 GLN B  76     4580   4521   4309    -50    -84    -22       N
ATOM   2250  N   THR B  77      20.251  18.533  50.552  1.00 35.00           N
ANISOU 2250  N   THR B  77     4352   4621   4325    111    170    -59       N
ATOM   2251  CA  THR B  77      19.118  18.487  49.624  1.00 35.59           C
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ANISOU 2251  CA  THR B  77     4537   4588   4398     78     43    -34       C
ATOM   2252  C   THR B  77      17.887  17.990  50.355  1.00 35.67           C
ANISOU 2252  C   THR B  77     4566   4511   4477     94     61    -58       C
ATOM   2253  O   THR B  77      18.005  17.366  51.415  1.00 35.20           O
ANISOU 2253  O   THR B  77     4453   4601   4320    146     77   -125       O
ATOM   2254  CB  THR B  77      19.423  17.436  48.530  1.00 36.24           C
ANISOU 2254  CB  THR B  77     4633   4648   4486     39     39    -72       C
ATOM   2255  OG1 THR B  77      19.518  16.150  49.150  1.00 35.57           O
ANISOU 2255  OG1 THR B  77     4498   4650   4369    101     88   -112       O
ATOM   2256  CG2 THR B  77      20.714  17.763  47.809  1.00 36.61           C
ANISOU 2256  CG2 THR B  77     4565   4790   4555     48     30    -88       C
ATOM   2257  N   PRO B  78      16.715  18.068  49.742  1.00 36.39           N
ANISOU 2257  N   PRO B  78     4685   4648   4495    129     -2    -20       N
ATOM   2258  CA  PRO B  78      15.493  17.506  50.292  1.00 37.02           C
ANISOU 2258  CA  PRO B  78     4681   4770   4615     65      7    -26       C
ATOM   2259  C   PRO B  78      15.638  16.001  50.513  1.00 39.10           C
ANISOU 2259  C   PRO B  78     5054   4873   4928    100     20     44       C
ATOM   2260  O   PRO B  78      15.197  15.402  51.502  1.00 38.80           O
ANISOU 2260  O   PRO B  78     4976   4916   4851    114     77    -16       O
ATOM   2261  CB  PRO B  78      14.450  17.807  49.222  1.00 36.04           C
ANISOU 2261  CB  PRO B  78     4715   4563   4416     58     55    -56       C
ATOM   2262  CG  PRO B  78      14.964  19.057  48.580  1.00 34.93           C
ANISOU 2262  CG  PRO B  78     4446   4572   4255     66     22    -74       C
ATOM   2263  CD  PRO B  78      16.464  18.800  48.464  1.00 36.11           C
ANISOU 2263  CD  PRO B  78     4519   4732   4469    124    -26    -47       C
ATOM   2264  N   GLU B  79      16.292  15.329  49.551  1.00 40.36           N
ANISOU 2264  N   GLU B  79     5193   5200   4942    148     52    -52       N
ATOM   2265  CA  GLU B  79      16.553  13.892  49.693  1.00 42.01           C
ANISOU 2265  CA  GLU B  79     5425   5273   5265    121    -12    -10       C
ATOM   2266  C   GLU B  79      17.416  13.645  50.928  1.00 41.29           C
ANISOU 2266  C   GLU B  79     5264   5245   5180    136     77    -70       C
ATOM   2267  O   GLU B  79      17.142  12.732  51.718  1.00 41.38           O
ANISOU 2267  O   GLU B  79     5311   5316   5095    188     71    -61       O
ATOM   2268  CB  GLU B  79      17.197  13.360  48.410  1.00 43.78           C
ANISOU 2268  CB  GLU B  79     5575   5681   5380     98     56    -94       C
ATOM   2269  CG  GLU B  79      17.521  11.876  48.491  1.00 46.12           C
ANISOU 2269  CG  GLU B  79     5937   5750   5836     60     -7    -31       C
ATOM   2270  CD  GLU B  79      18.321  11.381  47.292  1.00 47.70           C
ANISOU 2270  CD  GLU B  79     6102   6017   6006     83    100    -94       C
ATOM   2271  OE1 GLU B  79      19.353  11.964  46.902  1.00 47.99           O
ANISOU 2271  OE1 GLU B  79     6138   6021   6076    100    147    -99       O
ATOM   2272  OE2 GLU B  79      17.879  10.357  46.742  1.00 48.39           O
ANISOU 2272  OE2 GLU B  79     6172   6163   6052     17     62   -147       O
ATOM   2273  N   ASP B  80      18.438  14.456  51.169  1.00 40.72           N
ANISOU 2273  N   ASP B  80     5242   5181   5047    177     86    -87       N
ATOM   2274  CA  ASP B  80      19.270  14.336  52.362  1.00 40.90           C
ANISOU 2274  CA  ASP B  80     5181   5183   5177     92     27    -13       C
ATOM   2275  C   ASP B  80      18.447  14.311  53.655  1.00 41.39           C
ANISOU 2275  C   ASP B  80     5277   5258   5190    120     47     -7       C
ATOM   2276  O   ASP B  80      18.662  13.494  54.561  1.00 41.76           O
ANISOU 2276  O   ASP B  80     5337   5353   5177    202      6      4       O
ATOM   2277  CB  ASP B  80      20.255  15.505  52.434  1.00 40.50           C
ANISOU 2277  CB  ASP B  80     5105   5202   5082     79     58     -7       C
ATOM   2278  CG  ASP B  80      21.458  15.369  51.531  1.00 39.97           C
ANISOU 2278  CG  ASP B  80     5073   5096   5017     71     11    -31       C
ATOM   2279  OD1 ASP B  80      21.891  14.227  51.288  1.00 39.37           O
ANISOU 2279  OD1 ASP B  80     4979   5115   4866     95     39     -8       O
ATOM   2280  OD2 ASP B  80      22.002  16.390  51.058  1.00 40.19           O
ANISOU 2280  OD2 ASP B  80     5059   5128   5083    139     87    -18       O
ATOM   2281  N   LEU B  81      17.452  15.193  53.752  1.00 40.72           N
ANISOU 2281  N   LEU B  81     5205   5182   5085     94     35      6       N
ATOM   2282  CA  LEU B  81      16.604  15.338  54.931  1.00 39.97           C
ANISOU 2282  CA  LEU B  81     5058   5090   5039     54    -28     48       C
ATOM   2283  C   LEU B  81      15.333  14.528  54.960  1.00 39.64           C
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ANISOU 2283  C   LEU B  81     5037   5034   4991     88      4     70       C
ATOM   2284  O   LEU B  81      14.504  14.683  55.869  1.00 38.32           O
ANISOU 2284  O   LEU B  81     4836   4787   4938     92    -92    109       O
ATOM   2285  CB  LEU B  81      16.325  16.856  55.064  1.00 39.74           C
ANISOU 2285  CB  LEU B  81     5066   5109   4926     13     51    -42       C
ATOM   2286  CG  LEU B  81      17.616  17.650  55.337  1.00 39.96           C
ANISOU 2286  CG  LEU B  81     5045   5143   4994     -2     59     18       C
ATOM   2287  CD1 LEU B  81      17.503  19.114  54.972  1.00 40.36           C
ANISOU 2287  CD1 LEU B  81     5140   5111   5084     44     46    -41       C
ATOM   2288  CD2 LEU B  81      17.999  17.511  56.809  1.00 40.56           C
ANISOU 2288  CD2 LEU B  81     5128   5270   5015    -23     15    -53       C
ATOM   2289  N   ASP B  82      15.093  13.654  53.978  1.00 40.45           N
ANISOU 2289  N   ASP B  82     5185   5067   5115     74    -35     28       N
ATOM   2290  CA  ASP B  82      13.890  12.823  53.960  1.00 41.27           C
ANISOU 2290  CA  ASP B  82     5147   5240   5295     55    -43    -68       C
ATOM   2291  C   ASP B  82      12.610  13.641  53.846  1.00 38.94           C
ANISOU 2291  C   ASP B  82     5091   4877   4825    -39     -5      1       C
ATOM   2292  O   ASP B  82      11.569  13.350  54.437  1.00 38.51           O
ANISOU 2292  O   ASP B  82     5005   4892   4733    -45    -35    -82       O
ATOM   2293  CB  ASP B  82      13.903  11.949  55.217  1.00 44.41           C
ANISOU 2293  CB  ASP B  82     5763   5606   5506     71    -26     88       C
ATOM   2294  CG  ASP B  82      12.787  10.949  55.365  1.00 47.24           C
ANISOU 2294  CG  ASP B  82     5952   5986   6012   -102      2     16       C
ATOM   2295  OD1 ASP B  82      12.202  10.534  54.333  1.00 48.41           O
ANISOU 2295  OD1 ASP B  82     6186   6236   5971    -45     -5    -23       O
ATOM   2296  OD2 ASP B  82      12.442  10.561  56.505  1.00 48.88           O
ANISOU 2296  OD2 ASP B  82     6341   6238   5993    -28     15     14       O
ATOM   2297  N   MET B  83      12.661  14.741  53.092  1.00 36.91           N
ANISOU 2297  N   MET B  83     4787   4781   4457     75     -6    -95       N
ATOM   2298  CA  MET B  83      11.470  15.569  52.898  1.00 35.33           C
ANISOU 2298  CA  MET B  83     4651   4482   4292     -7     90    -43       C
ATOM   2299  C   MET B  83      10.453  14.882  51.998  1.00 36.41           C
ANISOU 2299  C   MET B  83     4689   4652   4493     29     10    -71       C
ATOM   2300  O   MET B  83      10.818  14.005  51.200  1.00 37.09           O
ANISOU 2300  O   MET B  83     4971   4677   4445      1      1   -132       O
ATOM   2301  CB  MET B  83      11.882  16.932  52.333  1.00 33.81           C
ANISOU 2301  CB  MET B  83     4343   4369   4133     84    -44    -86       C
ATOM   2302  CG  MET B  83      12.881  17.677  53.217  1.00 31.70           C
ANISOU 2302  CG  MET B  83     4195   4009   3839    140     80    -29       C
ATOM   2303  SD  MET B  83      13.259  19.326  52.606  1.00 31.16           S
ANISOU 2303  SD  MET B  83     4237   3999   3603    191     77    -73       S
ATOM   2304  CE  MET B  83      13.994  20.038  54.074  1.00 31.37           C
ANISOU 2304  CE  MET B  83     4141   4011   3766     96     11    -50       C
ATOM   2305  N   GLU B  84       9.183  15.224  52.135  1.00 36.04           N
ANISOU 2305  N   GLU B  84     4662   4593   4439    -52    -18   -109       N
ATOM   2306  CA  GLU B  84       8.084  14.752  51.318  1.00 35.35           C
ANISOU 2306  CA  GLU B  84     4504   4572   4356     29    -38     -2       C
ATOM   2307  C   GLU B  84       7.364  15.973  50.736  1.00 35.04           C
ANISOU 2307  C   GLU B  84     4491   4498   4322    -60    -45    -51       C
ATOM   2308  O   GLU B  84       7.447  17.076  51.253  1.00 33.52           O
ANISOU 2308  O   GLU B  84     4285   4465   3988     54   -109     42       O
ATOM   2309  CB  GLU B  84       7.055  13.905  52.049  1.00 35.95           C
ANISOU 2309  CB  GLU B  84     4539   4620   4501    -45    -58    -23       C
ATOM   2310  N   ASP B  85       6.648  15.721  49.639  1.00 34.60           N
ANISOU 2310  N   ASP B  85     4265   4627   4253     -3      2    -18       N
ATOM   2311  CA  ASP B  85       5.945  16.778  48.935  1.00 35.80           C
ANISOU 2311  CA  ASP B  85     4574   4602   4427     14     -8    -40       C
ATOM   2312  C   ASP B  85       5.078  17.603  49.870  1.00 34.39           C
ANISOU 2312  C   ASP B  85     4290   4555   4222    -54    -43     26       C
ATOM   2313  O   ASP B  85       4.333  17.101  50.719  1.00 33.99           O
ANISOU 2313  O   ASP B  85     4317   4566   4030   -146    -69   -109       O
ATOM   2314  CB  ASP B  85       5.139  16.090  47.819  1.00 37.12           C
ANISOU 2314  CB  ASP B  85     4608   4868   4626    -82    -71    -81       C
ATOM   2315  CG  ASP B  85       4.674  17.003  46.726  1.00 38.28           C
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ANISOU 2315  CG  ASP B  85     4901   4993   4651    -26    -13    -12       C
ATOM   2316  OD1 ASP B  85       5.322  18.024  46.401  1.00 37.59           O
ANISOU 2316  OD1 ASP B  85     4671   5044   4569    -58    -83   -118       O
ATOM   2317  OD2 ASP B  85       3.599  16.684  46.158  1.00 39.56           O
ANISOU 2317  OD2 ASP B  85     4901   5201   4928   -143     13    -79       O
ATOM   2318  N   ASN B  86       5.200  18.915  49.750  1.00 33.19           N
ANISOU 2318  N   ASN B  86     4126   4521   3966    -24   -112    -63       N
ATOM   2319  CA  ASN B  86       4.486  19.959  50.444  1.00 33.64           C
ANISOU 2319  CA  ASN B  86     4286   4460   4035     -3   -110    -50       C
ATOM   2320  C   ASN B  86       4.971  20.168  51.884  1.00 32.91           C
ANISOU 2320  C   ASN B  86     4150   4355   3998     33    -46    -96       C
ATOM   2321  O   ASN B  86       4.292  20.835  52.672  1.00 31.61           O
ANISOU 2321  O   ASN B  86     3942   4476   3592    -18   -182    -83       O
ATOM   2322  CB  ASN B  86       2.966  19.715  50.429  1.00 35.28           C
ANISOU 2322  CB  ASN B  86     4367   4624   4415      1    -63     -2       C
ATOM   2323  CG  ASN B  86       2.442  19.686  48.992  1.00 36.76           C
ANISOU 2323  CG  ASN B  86     4645   4833   4487     -8    -96    -37       C
ATOM   2324  OD1 ASN B  86       2.767  20.542  48.182  1.00 37.26           O
ANISOU 2324  OD1 ASN B  86     4795   4929   4432     38    -42    -24       O
ATOM   2325  ND2 ASN B  86       1.642  18.663  48.737  1.00 37.64           N
ANISOU 2325  ND2 ASN B  86     4948   4773   4579    -50    -59      2       N
ATOM   2326  N   ASP B  87       6.158  19.644  52.196  1.00 32.15           N
ANISOU 2326  N   ASP B  87     4132   4238   3843    -31    -77    -18       N
ATOM   2327  CA  ASP B  87       6.704  19.866  53.527  1.00 31.06           C
ANISOU 2327  CA  ASP B  87     4030   3998   3774   -112     20    -75       C
ATOM   2328  C   ASP B  87       7.021  21.344  53.685  1.00 30.65           C
ANISOU 2328  C   ASP B  87     4040   3998   3606    -34    -20    -63       C
ATOM   2329  O   ASP B  87       7.159  22.090  52.725  1.00 29.16           O
ANISOU 2329  O   ASP B  87     3780   3974   3324   -105   -114   -234       O
ATOM   2330  CB  ASP B  87       7.928  18.975  53.815  1.00 31.79           C
ANISOU 2330  CB  ASP B  87     4130   4088   3861    -62    -38     16       C
ATOM   2331  CG  ASP B  87       7.537  17.641  54.327  1.00 32.05           C
ANISOU 2331  CG  ASP B  87     4249   4050   3879    -68    -87    -69       C
ATOM   2332  OD1 ASP B  87       6.361  17.459  54.698  1.00 33.61           O
ANISOU 2332  OD1 ASP B  87     4358   4432   3980   -148     14    -89       O
ATOM   2333  OD2 ASP B  87       8.421  16.783  54.313  1.00 32.01           O
ANISOU 2333  OD2 ASP B  87     4192   4111   3859     -4   -251    -30       O
ATOM   2334  N   ILE B  88       7.179  21.725  54.967  1.00 29.57           N
ANISOU 2334  N   ILE B  88     3743   3903   3590     -9     58   -186       N
ATOM   2335  CA  ILE B  88       7.429  23.118  55.277  1.00 28.05           C
ANISOU 2335  CA  ILE B  88     3481   3766   3412    -14    133     39       C
ATOM   2336  C   ILE B  88       8.797  23.270  55.931  1.00 27.26           C
ANISOU 2336  C   ILE B  88     3530   3525   3302     14     67    -88       C
ATOM   2337  O   ILE B  88       9.174  22.471  56.778  1.00 28.03           O
ANISOU 2337  O   ILE B  88     3315   3848   3486    117    212    115       O
ATOM   2338  CB  ILE B  88       6.396  23.659  56.288  1.00 28.41           C
ANISOU 2338  CB  ILE B  88     3428   3859   3507     42     99    -37       C
ATOM   2339  CG1 ILE B  88       4.990  23.528  55.688  1.00 28.52           C
ANISOU 2339  CG1 ILE B  88     3543   3988   3307    -27     23    -25       C
ATOM   2340  CG2 ILE B  88       6.675  25.103  56.656  1.00 28.14           C
ANISOU 2340  CG2 ILE B  88     3510   3821   3361      6    127     43       C
ATOM   2341  CD1 ILE B  88       3.877  23.820  56.676  1.00 29.56           C
ANISOU 2341  CD1 ILE B  88     3529   4144   3559     69     95    -17       C
ATOM   2342  N   ILE B  89       9.483  24.324  55.524  1.00 26.67           N
ANISOU 2342  N   ILE B  89     3350   3743   3041     77    156     60       N
ATOM   2343  CA  ILE B  89      10.741  24.724  56.107  1.00 26.26           C
ANISOU 2343  CA  ILE B  89     3344   3526   3106    -45    110    -24       C
ATOM   2344  C   ILE B  89      10.468  25.988  56.897  1.00 26.67           C
ANISOU 2344  C   ILE B  89     3488   3568   3080     26      4      1       C
ATOM   2345  O   ILE B  89       9.939  26.938  56.324  1.00 27.18           O
ANISOU 2345  O   ILE B  89     3685   3667   2977    124    -46    -68       O
ATOM   2346  CB  ILE B  89      11.821  24.953  55.026  1.00 26.40           C
ANISOU 2346  CB  ILE B  89     3318   3507   3205    -31     57     -9       C
ATOM   2347  CG1 ILE B  89      12.107  23.586  54.379  1.00 26.98           C
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ANISOU 2347  CG1 ILE B  89     3411   3604   3237     46    116    -72       C
ATOM   2348  CG2 ILE B  89      13.054  25.557  55.646  1.00 24.42           C
ANISOU 2348  CG2 ILE B  89     3131   3182   2964     51     97    -16       C
ATOM   2349  CD1 ILE B  89      12.906  23.744  53.075  1.00 28.07           C
ANISOU 2349  CD1 ILE B  89     3552   3886   3226    -60     89     28       C
ATOM   2350  N   GLU B  90      10.839  25.973  58.188  1.00 24.16           N
ANISOU 2350  N   GLU B  90     3025   3221   2935     -2     33     23       N
ATOM   2351  CA  GLU B  90      10.607  27.175  58.989  1.00 24.49           C
ANISOU 2351  CA  GLU B  90     3225   3207   2871    -85     66     68       C
ATOM   2352  C   GLU B  90      11.857  28.035  59.003  1.00 24.52           C
ANISOU 2352  C   GLU B  90     3213   3201   2902    -45    -60    -23       C
ATOM   2353  O   GLU B  90      12.955  27.534  59.231  1.00 27.01           O
ANISOU 2353  O   GLU B  90     3227   3607   3429      8     69    -18       O
ATOM   2354  CB  GLU B  90      10.329  26.734  60.450  1.00 24.61           C
ANISOU 2354  CB  GLU B  90     3184   3296   2871    -32     61     48       C
ATOM   2355  CG  GLU B  90       9.076  25.871  60.526  1.00 25.59           C
ANISOU 2355  CG  GLU B  90     3121   3430   3170   -104    -87     -8       C
ATOM   2356  CD  GLU B  90       8.774  25.403  61.928  1.00 25.96           C
ANISOU 2356  CD  GLU B  90     3274   3335   3253   -120    -62     21       C
ATOM   2357  OE1 GLU B  90       9.683  25.438  62.787  1.00 26.78           O
ANISOU 2357  OE1 GLU B  90     3320   3461   3397    -99   -209    -65       O
ATOM   2358  OE2 GLU B  90       7.637  24.958  62.195  1.00 25.52           O
ANISOU 2358  OE2 GLU B  90     2889   3639   3166    -38   -142      9       O
ATOM   2359  N   ALA B  91      11.681  29.330  58.791  1.00 24.70           N
ANISOU 2359  N   ALA B  91     3094   3241   3049   -108     23     84       N
ATOM   2360  CA  ALA B  91      12.813  30.258  58.866  1.00 25.40           C
ANISOU 2360  CA  ALA B  91     3151   3299   3201   -140   -149     81       C
ATOM   2361  C   ALA B  91      12.744  30.993  60.200  1.00 26.48           C
ANISOU 2361  C   ALA B  91     3404   3548   3110     33    -80    128       C
ATOM   2362  O   ALA B  91      11.819  31.808  60.384  1.00 27.71           O
ANISOU 2362  O   ALA B  91     3475   3734   3321    126   -220     56       O
ATOM   2363  CB  ALA B  91      12.689  31.289  57.742  1.00 26.82           C
ANISOU 2363  CB  ALA B  91     3429   3610   3151    -21   -123    192       C
ATOM   2364  N   HIS B  92      13.708  30.727  61.091  1.00 25.06           N
ANISOU 2364  N   HIS B  92     3007   3421   3094   -168    -69     96       N
ATOM   2365  CA  HIS B  92      13.679  31.375  62.395  1.00 24.54           C
ANISOU 2365  CA  HIS B  92     3116   3121   3086      7    -76    165       C
ATOM   2366  C   HIS B  92      14.823  32.382  62.580  1.00 25.10           C
ANISOU 2366  C   HIS B  92     3187   3221   3130    -61    -92    160       C
ATOM   2367  O   HIS B  92      15.915  32.126  62.119  1.00 26.43           O
ANISOU 2367  O   HIS B  92     3207   3463   3374   -105   -109    265       O
ATOM   2368  CB  HIS B  92      13.949  30.292  63.471  1.00 24.59           C
ANISOU 2368  CB  HIS B  92     3147   3187   3007    -35    -22    205       C
ATOM   2369  CG  HIS B  92      12.860  29.284  63.631  1.00 23.34           C
ANISOU 2369  CG  HIS B  92     2871   3030   2966     90    -82     45       C
ATOM   2370  ND1 HIS B  92      11.964  29.387  64.667  1.00 23.67           N
ANISOU 2370  ND1 HIS B  92     2897   3055   3043    -29     -1    212       N
ATOM   2371  CD2 HIS B  92      12.531  28.172  62.948  1.00 22.65           C
ANISOU 2371  CD2 HIS B  92     2812   2915   2879     18   -113    157       C
ATOM   2372  CE1 HIS B  92      11.097  28.402  64.606  1.00 23.25           C
ANISOU 2372  CE1 HIS B  92     2936   3001   2894    -43   -101    -47       C
ATOM   2373  NE2 HIS B  92      11.407  27.627  63.574  1.00 23.09           N
ANISOU 2373  NE2 HIS B  92     2752   3110   2912     70    119     11       N
ATOM   2374  N   ARG B  93      14.566  33.443  63.319  1.00 25.17           N
ANISOU 2374  N   ARG B  93     3261   3157   3147     16   -168    226       N
ATOM   2375  CA  ARG B  93      15.564  34.440  63.679  1.00 26.29           C
ANISOU 2375  CA  ARG B  93     3264   3397   3329    -71   -179    285       C
ATOM   2376  C   ARG B  93      16.560  33.818  64.671  1.00 25.15           C
ANISOU 2376  C   ARG B  93     3218   3209   3128   -100    -80    232       C
ATOM   2377  O   ARG B  93      16.153  33.028  65.553  1.00 24.62           O
ANISOU 2377  O   ARG B  93     3068   3166   3121    -26    -56    327       O
ATOM   2378  CB  ARG B  93      14.765  35.572  64.320  1.00 30.02           C
ANISOU 2378  CB  ARG B  93     3881   3772   3754    103     38    150       C
ATOM   2379  CG  ARG B  93      15.472  36.824  64.747  1.00 35.79           C
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ANISOU 2379  CG  ARG B  93     4658   4347   4596   -231   -169      0       C
ATOM   2380  CD  ARG B  93      14.488  37.735  65.519  1.00 40.21           C
ANISOU 2380  CD  ARG B  93     5143   5015   5120    142     61      6       C
ATOM   2381  NE  ARG B  93      15.227  38.722  66.283  1.00 43.42           N
ANISOU 2381  NE  ARG B  93     5588   5369   5542    -81   -138    -12       N
ATOM   2382  CZ  ARG B  93      14.867  39.568  67.228  1.00 45.51           C
ANISOU 2382  CZ  ARG B  93     5870   5677   5744     49      7    -78       C
ATOM   2383  NH1 ARG B  93      13.612  39.655  67.659  1.00 46.68           N
ANISOU 2383  NH1 ARG B  93     5909   5935   5893     -9     45     14       N
ATOM   2384  NH2 ARG B  93      15.802  40.364  67.762  1.00 46.46           N
ANISOU 2384  NH2 ARG B  93     5921   5795   5937    -29    -27    -69       N
ATOM   2385  N   GLU B  94      17.835  34.154  64.532  1.00 24.37           N
ANISOU 2385  N   GLU B  94     3122   3107   3031     77     -9    220       N
ATOM   2386  CA  GLU B  94      18.881  33.732  65.481  1.00 23.40           C
ANISOU 2386  CA  GLU B  94     3098   2916   2878      4     20    217       C
ATOM   2387  C   GLU B  94      18.391  34.161  66.860  1.00 21.74           C
ANISOU 2387  C   GLU B  94     2883   2678   2697    -79    -97    290       C
ATOM   2388  O   GLU B  94      17.644  35.152  67.020  1.00 21.06           O
ANISOU 2388  O   GLU B  94     3010   2628   2365    -63    -18    350       O
ATOM   2389  CB  GLU B  94      20.226  34.432  65.247  1.00 27.46           C
ANISOU 2389  CB  GLU B  94     3263   3537   3633    -91    195    207       C
ATOM   2390  CG  GLU B  94      21.258  34.449  66.351  1.00 32.08           C
ANISOU 2390  CG  GLU B  94     4019   4147   4023    -45   -150    167       C
ATOM   2391  CD  GLU B  94      22.579  35.128  66.043  1.00 35.29           C
ANISOU 2391  CD  GLU B  94     4167   4527   4715   -120     74    160       C
ATOM   2392  OE1 GLU B  94      22.562  36.224  65.424  1.00 36.54           O
ANISOU 2392  OE1 GLU B  94     4394   4616   4872    -37    125    272       O
ATOM   2393  OE2 GLU B  94      23.695  34.650  66.419  1.00 36.86           O
ANISOU 2393  OE2 GLU B  94     4582   4548   4876     95     21    165       O
ATOM   2394  N   GLN B  95      18.801  33.366  67.875  1.00 19.64           N
ANISOU 2394  N   GLN B  95     2618   2349   2494    -82     46    174       N
ATOM   2395  CA  GLN B  95      18.424  33.720  69.241  1.00 18.66           C
ANISOU 2395  CA  GLN B  95     2531   2133   2427   -190    -26    154       C
ATOM   2396  C   GLN B  95      19.717  33.972  70.027  1.00 17.79           C
ANISOU 2396  C   GLN B  95     2290   2271   2199     -4     17    200       C
ATOM   2397  O   GLN B  95      20.686  33.195  69.891  1.00 19.08           O
ANISOU 2397  O   GLN B  95     2482   2421   2346     31   -243     66       O
ATOM   2398  CB  GLN B  95      17.664  32.611  70.007  1.00 17.94           C
ANISOU 2398  CB  GLN B  95     2313   2129   2376   -120    -69    166       C
ATOM   2399  CG  GLN B  95      16.305  32.372  69.311  1.00 18.66           C
ANISOU 2399  CG  GLN B  95     2334   2316   2438    -32   -176    240       C
ATOM   2400  CD  GLN B  95      15.559  31.171  69.883  1.00 20.08           C
ANISOU 2400  CD  GLN B  95     2645   2434   2552   -216    -34      7       C
ATOM   2401  OE1 GLN B  95      16.210  30.391  70.569  1.00 21.94           O
ANISOU 2401  OE1 GLN B  95     2934   2518   2883    -71      1    136       O
ATOM   2402  NE2 GLN B  95      14.280  31.092  69.613  1.00 20.24           N
ANISOU 2402  NE2 GLN B  95     2640   2405   2647     77    -81    173       N
ATOM   2403  N   ILE B  96      19.701  35.005  70.871  1.00 19.29           N
ANISOU 2403  N   ILE B  96     2494   2188   2646   -118    -79    139       N
ATOM   2404  CA  ILE B  96      20.823  35.279  71.764  1.00 19.53           C
ANISOU 2404  CA  ILE B  96     2611   2384   2424    -68      5     85       C
ATOM   2405  C   ILE B  96      20.254  35.486  73.178  1.00 18.46           C
ANISOU 2405  C   ILE B  96     2689   1956   2370     16     23    129       C
ATOM   2406  O   ILE B  96      19.038  35.698  73.361  1.00 17.67           O
ANISOU 2406  O   ILE B  96     2559   2087   2067     37     57     79       O
ATOM   2407  CB  ILE B  96      21.644  36.547  71.412  1.00 21.68           C
ANISOU 2407  CB  ILE B  96     2942   2501   2793   -144     82    117       C
ATOM   2408  CG1 ILE B  96      20.722  37.767  71.378  1.00 22.68           C
ANISOU 2408  CG1 ILE B  96     3119   2624   2873    -66     13    167       C
ATOM   2409  CG2 ILE B  96      22.289  36.340  70.046  1.00 24.38           C
ANISOU 2409  CG2 ILE B  96     3177   3023   3063   -232    295     23       C
ATOM   2410  CD1 ILE B  96      21.459  39.090  71.209  1.00 24.56           C
ANISOU 2410  CD1 ILE B  96     3550   2749   3034   -222     56     68       C
ATOM   2411  N   GLY B  97      21.127  35.430  74.181  1.00 17.64           N
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ANISOU 2411  N   GLY B  97     2402   1926   2374    -78     97     56       N
ATOM   2412  CA  GLY B  97      20.667  35.692  75.527  1.00 16.66           C
ANISOU 2412  CA  GLY B  97     2257   1869   2203     40   -122    173       C
ATOM   2413  C   GLY B  97      21.833  35.730  76.508  1.00 16.37           C
ANISOU 2413  C   GLY B  97     2346   1846   2027    -48     15     65       C
ATOM   2414  O   GLY B  97      22.844  35.095  76.262  1.00 15.60           O
ANISOU 2414  O   GLY B  97     2294   1889   1744     22    100     33       O
ATOM   2415  N   GLY B  98      21.589  36.477  77.568  1.00 15.68           N
ANISOU 2415  N   GLY B  98     2453   1617   1888   -159    135    180       N
ATOM   2416  CA  GLY B  98      22.595  36.730  78.598  1.00 16.42           C
ANISOU 2416  CA  GLY B  98     2469   1719   2050    -46     21     75       C
ATOM   2417  C   GLY B  98      22.176  35.984  79.863  1.00 16.46           C
ANISOU 2417  C   GLY B  98     2600   1615   2039    -96    -27    -56       C
ATOM   2418  O   GLY B  98      23.034  36.071  80.909  1.00 17.02           O
ANISOU 2418  O   GLY B  98     2479   1915   2071    132   -111     62       O
TER    2419      GLY B  98
HETATM 2420  O   HOH    1      19.651  30.058  83.232  1.00 17.25           O
ANISOU 2420  O   HOH    1     2472   1924   2157   -142    353   -122       O
HETATM 2421  O   HOH    2      19.243  26.284  69.954  1.00 19.68           O
ANISOU 2421  O   HOH    2     2524   2156   2796   -140     74    198       O
HETATM 2422  O   HOH    3      24.806  33.659  77.583  1.00 16.28           O
ANISOU 2422  O   HOH    3     2295   1881   2009    -78    238    120       O
HETATM 2423  O   HOH    4      35.539  13.854  89.780  1.00 27.42           O
ANISOU 2423  O   HOH    4     3329   2782   4306   -453   -173   -252       O
HETATM 2424  O   HOH    5      13.626  24.057  73.516  1.00 16.34           O
ANISOU 2424  O   HOH    5     2197   1908   2103    -56     25     16       O
HETATM 2425  O   HOH    6      19.889  20.307  63.946  1.00 24.27           O
ANISOU 2425  O   HOH    6     3109   3221   2889     93   -240     84       O
HETATM 2426  O   HOH    7      19.459  27.209  83.447  1.00 19.36           O
ANISOU 2426  O   HOH    7     3087   2146   2122    -11    454    219       O
HETATM 2427  O   HOH    8      36.110  32.059  76.728  1.00 20.80           O
ANISOU 2427  O   HOH    8     2587   2271   3045   -111   -177     46       O
HETATM 2428  O   HOH    9      39.603  34.562  74.994  1.00 25.42           O
ANISOU 2428  O   HOH    9     3037   2989   3634   -155    271   -117       O
HETATM 2429  O   HOH   10       7.319  15.790  68.932  1.00 23.05           O
ANISOU 2429  O   HOH   10     2891   3023   2845   -235    121   -301       O
HETATM 2430  O   HOH   11      36.269  31.500  79.570  1.00 24.80           O
ANISOU 2430  O   HOH   11     3213   3256   2953   -161   -343    -87       O
HETATM 2431  O   HOH   12      28.941  41.240  78.512  1.00 23.16           O
ANISOU 2431  O   HOH   12     3083   2195   3523    -76    314     91       O
HETATM 2432  O   HOH   13      13.566  17.047  65.780  1.00 26.41           O
ANISOU 2432  O   HOH   13     3433   3556   3045   -340   -104   -348       O
HETATM 2433  O   HOH   14      26.963  30.646  90.501  1.00 22.12           O
ANISOU 2433  O   HOH   14     3325   2856   2223   -319   -245   -104       O
HETATM 2434  O   HOH   15      37.785  24.360  80.585  1.00 24.25           O
ANISOU 2434  O   HOH   15     2761   3370   3083    482   -101     86       O
HETATM 2435  O   HOH   16      19.263  19.400  67.772  1.00 30.56           O
ANISOU 2435  O   HOH   16     3589   3688   4336   -126   -231     86       O
HETATM 2436  O   HOH   17      33.444  35.183  80.828  1.00 22.86           O
ANISOU 2436  O   HOH   17     3448   2497   2742    316   -292    219       O
HETATM 2437  O   HOH   18      19.956  21.117  86.302  1.00 23.06           O
ANISOU 2437  O   HOH   18     3394   2177   3190     43     28    175       O
HETATM 2438  O   HOH   19      12.619  17.491  86.136  1.00 29.62           O
ANISOU 2438  O   HOH   19     3541   3718   3996    -50     55    -99       O
HETATM 2439  O   HOH   20      13.054  28.919  73.370  1.00 20.76           O
ANISOU 2439  O   HOH   20     2517   2230   3140     18    -17    -64       O
HETATM 2440  O   HOH   21      35.696  38.599  74.730  1.00 22.85           O
ANISOU 2440  O   HOH   21     3062   2488   3132   -290    295   -364       O
HETATM 2441  O   HOH   22      24.135   9.921  89.518  1.00 30.44           O
ANISOU 2441  O   HOH   22     3960   3382   4226    285     12    -53       O
HETATM 2442  O   HOH   23       2.463   9.690  84.033  1.00 28.47           O
ANISOU 2442  O   HOH   23     3535   3243   4038   -675    -51     93       O
HETATM 2443  O   HOH   24      31.799  39.656  85.633  1.00 23.50           O
ANISOU 2443  O   HOH   24     3441   2251   3238   -157    -71     -8       O
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HETATM 2444  O   HOH    25      32.112  33.143  82.096  1.00 23.76           O
ANISOU 2444  O   HOH    25     3332   2950   2745    595    247    387       O
HETATM 2445  O   HOH    26       7.698  22.413  63.301  1.00 29.01           O
ANISOU 2445  O   HOH    26     3742   3973   3307     63     -5    279       O
HETATM 2446  O   HOH    27      14.534  34.761  85.038  1.00 26.28           O
ANISOU 2446  O   HOH    27     3462   2768   3757    473    100    -20       O
HETATM 2447  O   HOH    28      11.023  22.853  61.991  1.00 25.33           O
ANISOU 2447  O   HOH    28     3027   3163   3434    -78     96     41       O
HETATM 2448  O   HOH    29      22.313  30.321  59.892  1.00 39.42           O
ANISOU 2448  O   HOH    29     5046   5136   4797    -61     77    -36       O
HETATM 2449  O   HOH    30      31.490  17.266  66.262  1.00 24.59           O
ANISOU 2449  O   HOH    30     2982   3006   3355    -67    237   -316       O
HETATM 2450  O   HOH    31      27.364  41.768  84.190  1.00 26.32           O
ANISOU 2450  O   HOH    31     3256   2898   3847    -75    105    106       O
HETATM 2451  O   HOH    32      12.813  33.953  71.853  1.00 27.15           O
ANISOU 2451  O   HOH    32     3106   3587   3623     23   -590   -124       O
HETATM 2452  O   HOH    33      30.540  20.936  90.768  1.00 29.41           O
ANISOU 2452  O   HOH    33     3725   4009   3443    -67   -314    263       O
HETATM 2453  O   HOH    34      29.469   9.066  77.394  1.00 31.55           O
ANISOU 2453  O   HOH    34     4090   3174   4725    -10    -76     67       O
HETATM 2454  O   HOH    35       7.046   9.814  70.879  1.00 27.40           O
ANISOU 2454  O   HOH    35     3554   3351   3507    -30   -102   -126       O
HETATM 2455  O   HOH    36      11.781  34.052  64.099  1.00 26.97           O
ANISOU 2455  O   HOH    36     3606   3451   3191     -7   -188    104       O
HETATM 2456  O   HOH    37      13.747  32.917  67.074  1.00 25.84           O
ANISOU 2456  O   HOH    37     3150   3070   3599    138   -234     29       O
HETATM 2457  O   HOH    38      40.989  22.800  71.958  1.00 30.02           O
ANISOU 2457  O   HOH    38     3543   3952   3909    370    253   -161       O
HETATM 2458  O   HOH    39      35.724  20.786  64.481  1.00 31.70           O
ANISOU 2458  O   HOH    39     3747   4130   4169     41     54   -302       O
HETATM 2459  O   HOH    40      29.248  31.177  92.034  1.00 27.04           O
ANISOU 2459  O   HOH    40     3561   3525   3189     41    106    -52       O
HETATM 2460  O   HOH    41      16.731  19.308  68.657  1.00 23.24           O
ANISOU 2460  O   HOH    41     2932   2937   2962    -35     18   -260       O
HETATM 2461  O   HOH    42      11.592  31.817  65.888  1.00 29.89           O
ANISOU 2461  O   HOH    42     3548   4075   3733     54    315    103       O
HETATM 2462  O   HOH    43       9.517  22.269  59.558  1.00 24.82           O
ANISOU 2462  O   HOH    43     3149   3622   2660    111   -171    -88       O
HETATM 2463  O   HOH    44      15.935  10.353  84.557  1.00 30.61           O
ANISOU 2463  O   HOH    44     3701   3624   4304    -88    -58     18       O
HETATM 2464  O   HOH    45      28.604  41.191  88.587  1.00 28.52           O
ANISOU 2464  O   HOH    45     3662   3098   4075   -223    172     91       O
HETATM 2465  O   HOH    46      35.793  33.851  80.461  1.00 29.90           O
ANISOU 2465  O   HOH    46     3664   3710   3987     59    -40    237       O
HETATM 2466  O   HOH    47      40.058  25.649  81.260  1.00 33.89           O
ANISOU 2466  O   HOH    47     3757   4632   4485    -46   -155     80       O
HETATM 2467  O   HOH    48      17.335  25.487  46.362  1.00 36.44           O
ANISOU 2467  O   HOH    48     4492   4989   4366     92    344    122       O
HETATM 2468  O   HOH    49      35.363  39.486  72.192  1.00 33.90           O
ANISOU 2468  O   HOH    49     4422   4305   4152    -46   -124   -128       O
HETATM 2469  O   HOH    50      31.905  33.410  85.105  1.00 28.47           O
ANISOU 2469  O   HOH    50     4198   2777   3842    162   -364    -37       O
HETATM 2470  O   HOH    51      20.232   8.433  81.394  1.00 37.25           O
ANISOU 2470  O   HOH    51     4842   4543   4767     23    177    -76       O
HETATM 2471  O   HOH    52      23.343  22.748  60.568  1.00 30.09           O
ANISOU 2471  O   HOH    52     3582   4361   3489    160    -88   -116       O
HETATM 2472  O   HOH    53      22.966   9.616  83.135  1.00 31.32           O
ANISOU 2472  O   HOH    53     4181   3906   3815     76     59     -1       O
HETATM 2473  O   HOH    54      41.448  27.414  79.808  1.00 31.69           O
ANISOU 2473  O   HOH    54     3778   3902   4360    216   -132     74       O
HETATM 2474  O   HOH    55      18.977  18.912  87.579  1.00 27.87           O
ANISOU 2474  O   HOH    55     3544   3404   3643    -56     83    537       O
HETATM 2475  O   HOH    56      19.846  27.021  58.540  1.00 28.71           O
ANISOU 2475  O   HOH    56     3192   4150   3565    -46     62   -102       O
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HETATM 2476  O   HOH    57      18.893  38.381  68.300  1.00 39.18           O
ANISOU 2476  O   HOH    57    4835   5065   4988   -169   -131    302       O
HETATM 2477  O   HOH    58       6.902   8.651  82.704  1.00 28.45           O
ANISOU 2477  O   HOH    58    3411   3330   4067   -392   -302    113       O
HETATM 2478  O   HOH    59      17.849  16.715  86.154  1.00 29.54           O
ANISOU 2478  O   HOH    59    4120   3029   4077   -328   -270    384       O
HETATM 2479  O   HOH    60      33.565  14.842  76.735  1.00 27.80           O
ANISOU 2479  O   HOH    60    3718   2775   4069    220    139     28       O
HETATM 2480  O   HOH    61      31.434  37.317  86.923  1.00 29.54           O
ANISOU 2480  O   HOH    61    3467   4223   3531   -245     94    -71       O
HETATM 2481  O   HOH    63       8.212  24.757  92.578  1.00 33.84           O
ANISOU 2481  O   HOH    63    4422   4549   3887   -317    446    186       O
HETATM 2482  O   HOH    64       0.341  17.389  87.409  1.00 34.12           O
ANISOU 2482  O   HOH    64    4047   4436   4479     74     64     41       O
HETATM 2483  O   HOH    65      10.728  32.643  83.333  1.00 37.65           O
ANISOU 2483  O   HOH    65    4696   4580   5031    119     45   -165       O
HETATM 2484  O   HOH    66      25.977  41.295  79.529  1.00 38.48           O
ANISOU 2484  O   HOH    66    5182   4385   5052     10    -70    -13       O
HETATM 2485  O   HOH    67      -0.519  21.247  80.668  1.00 31.77           O
ANISOU 2485  O   HOH    67    3778   4088   4207     -6    141    -23       O
HETATM 2486  O   HOH    68      33.932  36.444  83.268  1.00 36.90           O
ANISOU 2486  O   HOH    68    4722   4842   4454     22   -181   -382       O
HETATM 2487  O   HOH    69      32.361  16.072  82.512  1.00 27.55           O
ANISOU 2487  O   HOH    69    3814   3115   3538    166    -85   -130       O
HETATM 2488  O   HOH    70      27.479  37.182  71.425  1.00 37.05           O
ANISOU 2488  O   HOH    70    5266   4168   4644    -49     94    223       O
HETATM 2489  O   HOH    71       5.892  25.721  64.244  1.00 31.68           O
ANISOU 2489  O   HOH    71    3672   4354   4009    -46     27    158       O
HETATM 2490  O   HOH    72       0.863  30.898  72.470  1.00 29.17           O
ANISOU 2490  O   HOH    72    3748   3817   3519    230   -173   -465       O
HETATM 2491  O   HOH    73      13.237  26.756  96.337  1.00 44.81           O
ANISOU 2491  O   HOH    73    5592   5719   5716   -119    125      4       O
HETATM 2492  O   HOH    74      25.614  12.403  81.897  1.00 32.99           O
ANISOU 2492  O   HOH    74    4047   4097   4391    273    -49   -168       O
HETATM 2493  O   HOH    75       0.392   7.960  83.650  1.00 44.90           O
ANISOU 2493  O   HOH    75    5506   5674   5881   -144     20   -128       O
HETATM 2494  O   HOH    76       2.842  20.053  90.559  1.00 33.42           O
ANISOU 2494  O   HOH    76    3790   4365   4544    -40    373    370       O
HETATM 2495  O   HOH    77      25.802  32.864  63.405  1.00 46.37           O
ANISOU 2495  O   HOH    77    6051   5780   5787    -48     51    212       O
HETATM 2496  O   HOH    78      20.698  17.182  89.026  1.00 28.05           O
ANISOU 2496  O   HOH    78    3497   3500   3659     76     72    370       O
HETATM 2497  O   HOH    79      27.986  17.672  91.656  1.00 35.19           O
ANISOU 2497  O   HOH    79    4901   3943   4528     90    -56    268       O
HETATM 2498  O   HOH    80      11.471  31.449  72.256  1.00 33.07           O
ANISOU 2498  O   HOH    80    3849   4128   4589   -305   -439   -386       O
HETATM 2499  O   HOH    81      17.541  19.065  35.838  1.00 36.53           O
ANISOU 2499  O   HOH    81    4680   4456   4742    -25    134    234       O
HETATM 2500  O   HOH    82       7.860   6.828  80.738  1.00 33.81           O
ANISOU 2500  O   HOH    82    4453   3990   4403   -357    -60    289       O
HETATM 2501  O   HOH    83      21.768  27.779  60.354  1.00 40.60           O
ANISOU 2501  O   HOH    83    4890   5315   5222     82    -54    -47       O
HETATM 2502  O   HOH    84      32.064  37.367  89.481  1.00 41.76           O
ANISOU 2502  O   HOH    84    5354   5268   5244     -7    -99    147       O
HETATM 2503  O   HOH    85       8.503   9.586  67.648  1.00 35.02           O
ANISOU 2503  O   HOH    85    4560   4198   4548   -151    -92    -68       O
HETATM 2504  O   HOH    86      35.055  16.029  80.808  1.00 30.32           O
ANISOU 2504  O   HOH    86    4584   3294   3640    -45    233    -30       O
HETATM 2505  O   HOH    87       6.989  13.177  66.266  1.00 33.80           O
ANISOU 2505  O   HOH    87    4125   3818   4898   -251    -63    -11       O
HETATM 2506  O   HOH    88      15.003  28.045  97.998  1.00 51.17           O
ANISOU 2506  O   HOH    88    6357   6627   6457     16    -15     -2       O
HETATM 2507  O   HOH    89      29.907  36.459  67.348  1.00 31.26           O
ANISOU 2507  O   HOH    89    4265   3612   3999   -117    198    -44       O
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HETATM 2508  O   HOH    90      10.674  27.500  42.469  1.00 43.25           O
ANISOU 2508  O   HOH    90     5645   5598   5190     95     86    -41       O
HETATM 2509  O   HOH    92      20.274  18.178  70.165  1.00 30.26           O
ANISOU 2509  O   HOH    92     3601   4289   3606   -159     23   -276       O
HETATM 2510  O   HOH    93      32.384  22.940  91.171  1.00 32.02           O
ANISOU 2510  O   HOH    93     3973   4057   4137   -113   -116    510       O
HETATM 2511  O   HOH    94      12.207  36.458  58.100  1.00 45.11           O
ANISOU 2511  O   HOH    94     5761   5563   5814    -38     46    -39       O
HETATM 2512  O   HOH    95      27.430  27.136  93.699  1.00 40.85           O
ANISOU 2512  O   HOH    95     5177   5242   5102     21     50     42       O
HETATM 2513  O   HOH    97      37.831  29.448  86.376  1.00 30.88           O
ANISOU 2513  O   HOH    97     4017   3710   4008   -175    -67     35       O
HETATM 2514  O   HOH    98      15.240  18.925  66.709  1.00 38.00           O
ANISOU 2514  O   HOH    98     4994   4738   4706     -7   -242    176       O
HETATM 2515  O   HOH    99       5.829  19.721  64.048  1.00 35.79           O
ANISOU 2515  O   HOH    99     4801   4416   4380   -274     19     66       O
HETATM 2516  O   HOH   101       6.090   6.593  72.934  1.00 39.21           O
ANISOU 2516  O   HOH   101     5096   4609   5195   -199    -38   -118       O
HETATM 2517  O   HOH   102      26.208  34.093  92.270  1.00 34.48           O
ANISOU 2517  O   HOH   102     4658   4274   4169     10   -114   -190       O
HETATM 2518  O   HOH   103      19.304  37.782  81.584  1.00 42.00           O
ANISOU 2518  O   HOH   103     5191   5317   5451    114     35      0       O
HETATM 2519  O   HOH   104      10.583  32.305  86.587  1.00 39.73           O
ANISOU 2519  O   HOH   104     4880   4948   5265    115    208   -302       O
HETATM 2520  O   HOH   105       4.086   7.006  74.602  1.00 42.19           O
ANISOU 2520  O   HOH   105     5191   5231   5610   -135   -123    -43       O
HETATM 2521  O   HOH   106      36.699  40.392  83.292  1.00 44.11           O
ANISOU 2521  O   HOH   106     5779   5365   5616    119     20    287       O
HETATM 2522  O   HOH   107      17.276  37.421  90.299  1.00 40.27           O
ANISOU 2522  O   HOH   107     5148   4767   5385    -33     -7    -97       O
HETATM 2523  O   HOH   108      30.148  37.356  69.897  1.00 35.36           O
ANISOU 2523  O   HOH   108     4787   4293   4354    -46    184    242       O
HETATM 2524  O   HOH   109      20.050  11.270  82.593  1.00 30.97           O
ANISOU 2524  O   HOH   109     3907   3736   4126   -397   -192   -331       O
HETATM 2525  O   HOH   110      32.982  18.621  61.866  1.00 40.10           O
ANISOU 2525  O   HOH   110     5006   5145   5083    -75     -7   -109       O
HETATM 2526  O   HOH   111      31.183  44.426  71.705  1.00 38.92           O
ANISOU 2526  O   HOH   111     5834   4043   4912    117   -199   -112       O
HETATM 2527  O   HOH   112      19.410  35.437  91.026  1.00 31.27           O
ANISOU 2527  O   HOH   112     4105   3674   4102     20   -307     -1       O
HETATM 2528  O   HOH   113      10.508  34.816  74.376  1.00 35.06           O
ANISOU 2528  O   HOH   113     4113   4123   5085     46   -303      5       O
HETATM 2529  O   HOH   114      -1.049  11.092  82.134  1.00 40.12           O
ANISOU 2529  O   HOH   114     4844   4782   5618   -315     69   -108       O
HETATM 2530  O   HOH   115      19.897   5.671  74.532  1.00 36.57           O
ANISOU 2530  O   HOH   115     5109   4121   4665     66     99   -313       O
HETATM 2531  O   HOH   116      12.797  36.998  68.353  1.00 44.20           O
ANISOU 2531  O   HOH   116     5407   5654   5732     -9     11    -23       O
HETATM 2532  O   HOH   117      37.204  16.913  77.312  1.00 42.42           O
ANISOU 2532  O   HOH   117     5547   5241   5330     35    136    -64       O
HETATM 2533  O   HOH   118      24.098  26.614  55.883  1.00 46.04           O
ANISOU 2533  O   HOH   118     5820   5869   5803   -112    -31     92       O
HETATM 2534  O   HOH   119       9.740   7.380  78.924  1.00 35.49           O
ANISOU 2534  O   HOH   119     4494   4049   4943   -286    -98   -193       O
HETATM 2535  O   HOH   120      26.325  10.188  80.789  1.00 36.65           O
ANISOU 2535  O   HOH   120     4396   4867   4661    -85    174   -265       O
HETATM 2536  O   HOH   121      24.800   8.376  81.628  1.00 36.20           O
ANISOU 2536  O   HOH   121     4413   4540   4803     33   -114   -123       O
HETATM 2537  O   HOH   122       0.529  25.300  65.097  1.00 30.84           O
ANISOU 2537  O   HOH   122     4482   3825   3412    -21     85      5       O
HETATM 2538  O   HOH   123      16.009  22.094  95.421  1.00 37.78           O
ANISOU 2538  O   HOH   123     4667   5104   4586    -25     39     87       O
HETATM 2539  O   HOH   124      42.684  19.628  77.757  1.00 34.07           O
ANISOU 2539  O   HOH   124     4309   4247   4388    254   -218     92       O
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HETATM 2540  O   HOH   125      35.783  23.733  86.601  1.00 36.64           O
ANISOU 2540  O   HOH   125    4533   4858   4530     67    -40    -85       O
HETATM 2541  O   HOH   126      21.796  40.661  81.020  1.00 29.22           O
ANISOU 2541  O   HOH   126    4192   3615   3294    121   -111   -252       O
HETATM 2542  O   HOH   127      19.560  40.153  79.738  1.00 34.02           O
ANISOU 2542  O   HOH   127    4065   4328   4535     11    243   -240       O
HETATM 2543  O   HOH   128      24.074  40.355  87.308  1.00 36.13           O
ANISOU 2543  O   HOH   128    4930   4116   4679     -9     40   -138       O
HETATM 2544  O   HOH   129       9.039  32.249  66.343  1.00 32.45           O
ANISOU 2544  O   HOH   129    3876   4369   4085     79     91    152       O
HETATM 2545  O   HOH   130      12.440  34.199  86.784  1.00 39.42           O
ANISOU 2545  O   HOH   130    4746   5219   5013     65    187   -163       O
HETATM 2546  O   HOH   132      18.577  41.151  72.469  1.00 40.69           O
ANISOU 2546  O   HOH   132    5132   5116   5212   -131     38    175       O
HETATM 2547  O   HOH   133      26.035  17.547  59.645  1.00 37.43           O
ANISOU 2547  O   HOH   133    4588   4901   4733     41     -7    -48       O
HETATM 2548  O   HOH   134       6.841  27.863  88.767  1.00 43.13           O
ANISOU 2548  O   HOH   134    5586   5488   5312    -99   -198     85       O
HETATM 2549  O   HOH   135       5.747  24.462  60.265  1.00 31.64           O
ANISOU 2549  O   HOH   135    3794   4365   3864   -157   -132    -29       O
HETATM 2550  O   HOH   136       5.347  31.806  46.511  1.00 34.07           O
ANISOU 2550  O   HOH   136    4493   4356   4098    306   -297     88       O
HETATM 2551  O   HOH   137      22.102   8.719  85.540  1.00 35.29           O
ANISOU 2551  O   HOH   137    4212   4737   4457    -50    118     -7       O
HETATM 2552  O   HOH   138      21.348  33.060  45.448  1.00 50.48           O
ANISOU 2552  O   HOH   138    6358   6409   6412    -24     89    -14       O
HETATM 2553  O   HOH   139      21.196  38.672  66.903  1.00 38.48           O
ANISOU 2553  O   HOH   139    4950   4534   5139    -44    180    282       O
HETATM 2554  O   HOH   140      19.595  17.890  37.318  1.00 42.21           O
ANISOU 2554  O   HOH   140    5649   5133   5254    -91      9     18       O
HETATM 2555  O   HOH   141      17.506  17.570  66.106  1.00 46.57           O
ANISOU 2555  O   HOH   141    5703   6043   5950   -156    -14    -25       O
HETATM 2556  O   HOH   142      37.768  20.451  86.955  1.00 39.70           O
ANISOU 2556  O   HOH   142    4699   5282   5103     57   -225     95       O
HETATM 2557  O   HOH   144      20.596  25.321  45.223  1.00 40.73           O
ANISOU 2557  O   HOH   144    5073   5370   5033     60     83     12       O
HETATM 2558  O   HOH   145      24.915  20.661  59.526  1.00 32.65           O
ANISOU 2558  O   HOH   145    4431   4051   3925    -44    -70    -36       O
HETATM 2559  O   HOH   146      23.130  25.120  59.370  1.00 32.05           O
ANISOU 2559  O   HOH   146    3775   4339   4063    220    207     83       O
HETATM 2560  O   HOH   147      15.211  22.046  92.930  1.00 38.03           O
ANISOU 2560  O   HOH   147    4653   4976   4819      5    -16    221       O
HETATM 2561  O   HOH   148       3.874   5.766  77.070  1.00 45.93           O
ANISOU 2561  O   HOH   148    5735   5794   5921    146    -74     72       O
HETATM 2562  O   HOH   149      39.692  16.148  81.822  1.00 42.50           O
ANISOU 2562  O   HOH   149    5244   5204   5700    150    -53      7       O
HETATM 2563  O   HOH   150      28.544  29.691  94.309  1.00 45.60           O
ANISOU 2563  O   HOH   150    5856   5761   5709    -69     12     11       O
HETATM 2564  O   HOH   151      15.761  28.212  88.984  1.00 33.46           O
ANISOU 2564  O   HOH   151    4658   4153   3901   -163    268    362       O
HETATM 2565  O   HOH   152       3.456  35.442  52.303  1.00 40.94           O
ANISOU 2565  O   HOH   152    5075   5208   5272    260   -207     13       O
HETATM 2566  O   HOH   153      38.432  31.309  63.732  1.00 54.84           O
ANISOU 2566  O   HOH   153    6983   6977   6877     87    -54   -132       O
HETATM 2567  O   HOH   154      45.567  30.031  75.704  1.00 48.83           O
ANISOU 2567  O   HOH   154    6039   6212   6304    -60     37    -69       O
HETATM 2568  O   HOH   155       5.351   7.890  70.467  1.00 34.90           O
ANISOU 2568  O   HOH   155    4391   4202   4666    -41   -141    -86       O
HETATM 2569  O   HOH   156       5.248  12.467  63.713  1.00 49.93           O
ANISOU 2569  O   HOH   156    6398   6210   6364    -98    -91    -20       O
HETATM 2570  O   HOH   157      19.804  12.771  80.652  1.00 38.88           O
ANISOU 2570  O   HOH   157    4912   4876   4986   -111     -2   -195       O
HETATM 2571  O   HOH   158      24.298  27.085  62.174  1.00 37.61           O
ANISOU 2571  O   HOH   158    5032   4699   4558    209    198      5       O
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HETATM 2572  O   HOH   159      -2.754  18.937  70.168  1.00 49.15           O
ANISOU 2572  O   HOH   159     6055   6297   6322    135    -27    -66       O
HETATM 2573  O   HOH   160      20.325   9.737  74.178  1.00 33.76           O
ANISOU 2573  O   HOH   160     4095   4137   4594    -44    180   -237       O
HETATM 2574  O   HOH   161       4.663  27.190  59.648  1.00 44.33           O
ANISOU 2574  O   HOH   161     5691   5924   5227    128     -4    114       O
HETATM 2575  O   HOH   162      36.688  13.560  67.532  1.00 45.15           O
ANISOU 2575  O   HOH   162     5819   5609   5729    -39      5     64       O
HETATM 2576  O   HOH   163      17.051  29.122  91.358  1.00 43.44           O
ANISOU 2576  O   HOH   163     5359   5484   5663   -185     60     22       O
HETATM 2577  O   HOH   164      19.304  17.699  64.312  1.00 34.62           O
ANISOU 2577  O   HOH   164     4486   4139   4530      8     46    -91       O
HETATM 2578  O   HOH   165       4.437  33.730  48.186  1.00 44.78           O
ANISOU 2578  O   HOH   165     5530   5789   5697    192   -103     47       O
HETATM 2579  O   HOH   166      19.582  15.633  67.366  1.00 39.27           O
ANISOU 2579  O   HOH   166     5095   4943   4884     41    307    -86       O
HETATM 2580  O   HOH   167       3.313  25.443  63.514  1.00 35.90           O
ANISOU 2580  O   HOH   167     4498   4592   4549      4    -51    116       O
HETATM 2581  O   HOH   168      29.036  33.803  92.215  1.00 37.42           O
ANISOU 2581  O   HOH   168     4880   4260   5077    229    -77     84       O
HETATM 2582  O   HOH   169      27.439  37.535  67.031  1.00 49.94           O
ANISOU 2582  O   HOH   169     6490   6199   6285     67     81     45       O
HETATM 2583  O   HOH   170      39.359  22.141  64.730  1.00 39.59           O
ANISOU 2583  O   HOH   170     4994   4958   5090    -66    172     89       O
HETATM 2584  O   HOH   171       2.618  29.140  76.067  1.00 40.90           O
ANISOU 2584  O   HOH   171     5201   5034   5304     72    -24     42       O
HETATM 2585  O   HOH   172      19.141  42.727  78.598  1.00 44.77           O
ANISOU 2585  O   HOH   172     5768   5454   5789    104     93   -108       O
HETATM 2586  O   HOH   173      26.708  12.693  66.306  1.00 51.60           O
ANISOU 2586  O   HOH   173     6466   6618   6521   -185    -11    -61       O
HETATM 2587  O   HOH   174      14.550   4.591  79.369  1.00 54.16           O
ANISOU 2587  O   HOH   174     6803   6773   7001     24    -63     39       O
HETATM 2588  O   HOH   175       3.502  23.110  48.771  1.00 45.77           O
ANISOU 2588  O   HOH   175     5770   5943   5677    -13    -56     -2       O
HETATM 2589  O   HOH   176      21.028  19.774  93.260  1.00 35.01           O
ANISOU 2589  O   HOH   176     4493   4631   4180   -114    312    224       O
HETATM 2590  O   HOH   177      37.317  15.925  74.887  1.00 47.41           O
ANISOU 2590  O   HOH   177     6282   5883   5849    146     -6   -112       O
HETATM 2591  O   HOH   178       5.970  20.098  57.147  1.00 43.65           O
ANISOU 2591  O   HOH   178     5579   5670   5334    112    -43    188       O
HETATM 2592  O   HOH   180      31.762   9.526  70.915  1.00 42.55           O
ANISOU 2592  O   HOH   180     5672   5064   5430   -172     83    105       O
HETATM 2593  O   HOH   181      47.822  24.554  70.761  1.00 41.72           O
ANISOU 2593  O   HOH   181     5177   5233   5440    136     63    -20       O
HETATM 2594  O   HOH   182      26.734  24.919  50.172  1.00 52.79           O
ANISOU 2594  O   HOH   182     6486   6848   6723     28    117     23       O
HETATM 2595  O   HOH   183      32.925  11.685  69.753  1.00 42.43           O
ANISOU 2595  O   HOH   183     5774   4874   5474     65    -12    -10       O
HETATM 2596  O   HOH   184      18.971  15.202  87.889  1.00 38.16           O
ANISOU 2596  O   HOH   184     4719   4617   5163     37    175    -86       O
HETATM 2597  O   HOH   185      35.218  26.224  90.859  1.00 49.60           O
ANISOU 2597  O   HOH   185     6211   6225   6412    -62     76     80       O
HETATM 2598  O   HOH   186       5.227  24.542  47.195  1.00 43.45           O
ANISOU 2598  O   HOH   186     5439   5733   5336     59      4      7       O
HETATM 2599  O   HOH   187      39.009  31.723  80.027  1.00 34.64           O
ANISOU 2599  O   HOH   187     4598   4576   3987   -233    -35   -224       O
HETATM 2600  O   HOH   188      42.214  26.523  66.397  1.00 42.66           O
ANISOU 2600  O   HOH   188     5557   5491   5160    179    231    -83       O
HETATM 2601  O   HOH   189      17.465  32.770  93.454  1.00 51.95           O
ANISOU 2601  O   HOH   189     6708   6623   6405     16    138     95       O
HETATM 2602  O   HOH   190       8.735  15.447  39.420  1.00 54.50           O
ANISOU 2602  O   HOH   190     6832   6858   7019      0    -35      6       O
HETATM 2603  O   HOH   191      -2.607  20.239  72.368  1.00 40.07           O
ANISOU 2603  O   HOH   191     4840   5063   5323     14    141     81       O
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HETATM 2604  O   HOH   193      33.794  37.511  70.614  1.00 42.65           O
ANISOU 2604  O   HOH   193    5608   5288   5308    145    -43    -58       O
HETATM 2605  O   HOH   195       3.507  13.927  50.971  1.00 59.90           O
ANISOU 2605  O   HOH   195    7570   7678   7511      0      2      8       O
HETATM 2606  O   HOH   196      -4.736  20.639  73.512  1.00 40.93           O
ANISOU 2606  O   HOH   196    5209   4993   5352    -36   -222     85       O
HETATM 2607  O   HOH   197      26.092  19.633  55.216  1.00 51.00           O
ANISOU 2607  O   HOH   197    6169   6535   6675     44    -10   -122       O
HETATM 2608  O   HOH   198      23.781  30.889  93.836  1.00 32.97           O
ANISOU 2608  O   HOH   198    4468   4241   3820    -47    -78    114       O
HETATM 2609  O   HOH   200      21.093  30.159  56.807  1.00 52.30           O
ANISOU 2609  O   HOH   200    6449   6810   6614     70    103    -34       O
HETATM 2610  O   HOH   201       6.287  28.496  61.060  1.00 47.40           O
ANISOU 2610  O   HOH   201    6270   5946   5795    178     56    -66       O
HETATM 2611  O   HOH   202      -1.544  13.525  70.641  1.00 37.09           O
ANISOU 2611  O   HOH   202    4297   4780   5016   -377   -349    -40       O
HETATM 2612  O   HOH   203       7.553  20.917  60.941  1.00 47.92           O
ANISOU 2612  O   HOH   203    5823   6106   6279   -110     66    -11       O
HETATM 2613  O   HOH   204      17.614  21.404  91.766  1.00 39.24           O
ANISOU 2613  O   HOH   204    4982   4967   4958    -68    115    139       O
HETATM 2614  O   HOH   205       3.511  31.591  63.721  1.00 50.48           O
ANISOU 2614  O   HOH   205    6487   6369   6325    132    -63     48       O
HETATM 2615  O   HOH   206      32.461  39.367  68.538  1.00 60.12           O
ANISOU 2615  O   HOH   206    7617   7556   7670     25    -55    -82       O
HETATM 2616  O   HOH   207      27.566  32.440  60.770  1.00 45.93           O
ANISOU 2616  O   HOH   207    5774   5890   5788     -5   -119     49       O
HETATM 2617  O   HOH   208      17.698  37.711  66.116  1.00 40.56           O
ANISOU 2617  O   HOH   208    5267   4922   5224     87     46    245       O
HETATM 2618  O   HOH   209       1.483  26.616  79.265  1.00 54.08           O
ANISOU 2618  O   HOH   209    6873   6913   6760    -24     39     66       O
HETATM 2619  O   HOH   210      42.034  27.866  63.967  1.00 56.30           O
ANISOU 2619  O   HOH   210    7077   7232   7083    108     36    -14       O
HETATM 2620  O   HOH   211      43.429  19.817  70.829  1.00 50.34           O
ANISOU 2620  O   HOH   211    6362   6386   6381     14    -97    -26       O
HETATM 2621  O   HOH   212      37.808  23.533  62.993  1.00 40.32           O
ANISOU 2621  O   HOH   212    4939   5295   5086   -122    154    -65       O
HETATM 2622  O   HOH   213      43.082  31.381  78.491  1.00 56.01           O
ANISOU 2622  O   HOH   213    7107   7033   7141    -44    -49    -85       O
HETATM 2623  O   HOH   215      11.830   4.624  80.523  1.00 55.43           O
ANISOU 2623  O   HOH   215    6901   6996   7162    -35    -13     76       O
HETATM 2624  O   HOH   216      15.166  16.314  86.736  1.00 38.36           O
ANISOU 2624  O   HOH   216    4438   5215   4921   -232     43     30       O
HETATM 2625  O   HOH   217      36.377  16.002  72.427  1.00 35.99           O
ANISOU 2625  O   HOH   217    5335   3766   4575    -14    -14     33       O
HETATM 2626  O   HOH   218      -1.373  11.869  79.645  1.00 41.53           O
ANISOU 2626  O   HOH   218    4912   5117   5751   -296   -120     20       O
HETATM 2627  O   HOH   219      -3.379  16.353  86.986  1.00 45.74           O
ANISOU 2627  O   HOH   219    5715   5830   5833     85     17    -43       O
HETATM 2628  O   HOH   220       2.091   6.405  72.737  1.00 50.82           O
ANISOU 2628  O   HOH   220    6364   6358   6589    -22    -48     13       O
HETATM 2629  O   HOH   221       2.920  10.850  69.175  1.00 45.38           O
ANISOU 2629  O   HOH   221    5809   5558   5877    -19    -81    -71       O
HETATM 2630  O   HOH   222       5.981  25.400  90.850  1.00 57.36           O
ANISOU 2630  O   HOH   222    7302   7230   7264     43     55    -27       O
HETATM 2631  O   HOH   224      16.947  25.759  97.908  1.00 45.97           O
ANISOU 2631  O   HOH   224    5585   6066   5815     81     93     -5       O
HETATM 2632  O   HOH   225      19.414  21.824  39.526  1.00 53.64           O
ANISOU 2632  O   HOH   225    6777   6754   6848    -44     50    -87       O
HETATM 2633  O   HOH   226       1.800  25.637  74.624  1.00 40.30           O
ANISOU 2633  O   HOH   226    4930   5253   5128   -148    144    -70       O
HETATM 2634  O   HOH   227      23.269  14.956  55.180  1.00 48.49           O
ANISOU 2634  O   HOH   227    6018   6304   6101     89    -65    -63       O
HETATM 2635  O   HOH   228      18.568  32.106  45.086  1.00 45.28           O
ANISOU 2635  O   HOH   228    5629   5870   5706    135    119     94       O
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HETATM 2636  O   HOH   229      18.157  28.244  94.243  1.00 43.77           O
ANISOU 2636  O   HOH   229    5417   5624   5591     14    -48   -195       O
HETATM 2637  O   HOH   231       3.941   5.319  83.232  1.00 58.77           O
ANISOU 2637  O   HOH   231    7480   7292   7557    -68    -12     33       O
HETATM 2638  O   HOH   233      23.872  43.243  83.729  1.00 49.18           O
ANISOU 2638  O   HOH   233    6397   6031   6259    -26     20     45       O
HETATM 2639  O   HOH   234       5.807  35.953  86.478  1.00 39.50           O
ANISOU 2639  O   HOH   234    5214   4636   5158    168    -47   -181       O
HETATM 2640  O   HOH   235      -1.318   9.821  84.486  1.00 62.05           O
ANISOU 2640  O   HOH   235    7811   7836   7927    -63    -30     13       O
HETATM 2641  O   HOH   236       1.804  32.375  90.178  1.00 56.49           O
ANISOU 2641  O   HOH   236    7043   7190   7232    -12    -52      5       O
HETATM 2642  O   HOH   237      -0.925  21.448  82.987  1.00 39.99           O
ANISOU 2642  O   HOH   237    4850   5256   5088    -36    -37     75       O
HETATM 2643  O   HOH   239       2.879   8.457  71.154  1.00 47.58           O
ANISOU 2643  O   HOH   239    6000   5881   6197   -102    -52    -53       O
HETATM 2644  O   HOH   240      18.732  39.891  89.712  1.00 45.92           O
ANISOU 2644  O   HOH   240    5949   5499   5997     25    -30    -26       O
HETATM 2645  O   HOH   241      25.660  28.109  50.609  1.00 51.03           O
ANISOU 2645  O   HOH   241    6333   6478   6578   -120     99     67       O
HETATM 2646  O   HOH   244      38.699  32.712  88.082  1.00 56.52           O
ANISOU 2646  O   HOH   244    7097   7278   7100    -62      6     26       O
HETATM 2647  O   HOH   245      18.200  11.032  69.905  1.00 55.67           O
ANISOU 2647  O   HOH   245    7037   7069   7046     47     -6    -62       O
HETATM 2648  O   HOH   247       6.266  30.766  77.520  1.00 35.27           O
ANISOU 2648  O   HOH   247    4116   4315   4970    335    103     -7       O
HETATM 2649  O   HOH   248      10.443  35.367  90.850  1.00 38.88           O
ANISOU 2649  O   HOH   248    4926   4982   4866    -35     46    -99       O
HETATM 2650  O   HOH   249      34.849  11.886  63.661  1.00 58.13           O
ANISOU 2650  O   HOH   249    7371   7310   7407     12    -53     -1       O
HETATM 2651  O   HOH   250      -0.751  29.875  55.099  1.00 52.77           O
ANISOU 2651  O   HOH   250    6498   6850   6703    -17     61     16       O
HETATM 2652  O   HOH   251      39.775  29.228  84.737  1.00 44.55           O
ANISOU 2652  O   HOH   251    5394   5624   5909    -51    -95      5       O
HETATM 2653  O   HOH   252       8.905  31.517  73.237  1.00 31.68           O
ANISOU 2653  O   HOH   252    3599   4161   4276    -13    -92    199       O
HETATM 2654  O   HOH   253       5.904   5.392  79.575  1.00 44.36           O
ANISOU 2654  O   HOH   253    5611   5491   5754   -110    117    -17       O
HETATM 2655  O   HOH   254       2.593  27.491  57.553  1.00 61.05           O
ANISOU 2655  O   HOH   254    7747   7802   7645     56    -70     19       O
HETATM 2656  O   HOH   255      -3.034   6.388  73.651  1.00 41.01           O
ANISOU 2656  O   HOH   255    5096   5113   5373   -260    -71     37       O
HETATM 2657  O   HOH   256      15.248  11.098  45.922  1.00 49.92           O
ANISOU 2657  O   HOH   256    6452   6259   6256    -26    -12     -3       O
HETATM 2658  O   HOH   257      20.586  23.871  40.837  1.00 47.02           O
ANISOU 2658  O   HOH   257    5988   6052   5825    -38    -22    -76       O
HETATM 2659  O   HOH   258      10.220  32.449  75.430  1.00 44.35           O
ANISOU 2659  O   HOH   258    5310   5676   5867    -52     22    -83       O
HETATM 2660  O   HOH   259      20.623  15.671  38.604  1.00 48.71           O
ANISOU 2660  O   HOH   259    6276   6190   6043    -78     24     29       O
HETATM 2661  O   HOH   260      49.148  22.270  79.979  1.00 47.07           O
ANISOU 2661  O   HOH   260    5736   6174   5974     40    -50    112       O
HETATM 2662  O   HOH   261       9.316  33.141  94.966  1.00 57.50           O
ANISOU 2662  O   HOH   261    7324   7233   7291     58    115    -26       O
HETATM 2663  O   HOH   262      29.350  38.956  63.364  1.00 53.03           O
ANISOU 2663  O   HOH   262    6704   6705   6739     -9     35     82       O
HETATM 2664  O   HOH   263      49.220  20.731  77.265  1.00 54.08           O
ANISOU 2664  O   HOH   263    6622   6961   6967     62    -33    -45       O
HETATM 2665  O   HOH   265       4.082  31.314  76.389  1.00 43.10           O
ANISOU 2665  O   HOH   265    5426   5400   5548     40     86    -68       O
HETATM 2666  O   HOH   266       8.276  32.415  76.974  1.00 48.92           O
ANISOU 2666  O   HOH   266    5978   6294   6317    -38     21     23       O
HETATM 2667  O   HOH   267       8.287  33.166  63.785  1.00 45.99           O
ANISOU 2667  O   HOH   267    5603   6034   5836     13    -41     21       O
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HETATM 2668  O   HOH   269      -3.983   4.553  75.511  1.00 45.68           O
ANISOU 2668  O   HOH   269    5671   5698   5986   -289      4     -5       O
HETATM 2669  O   HOH   271      13.110  14.292  49.307  1.00 45.73           O
ANISOU 2669  O   HOH   271    5983   5656   5736    -77    -50     33       O
HETATM 2670  O   HOH   272      42.217  40.987  61.064  1.00 53.96           O
ANISOU 2670  O   HOH   272    6816   6807   6881    -17    122     51       O
HETATM 2671  O   HOH   275      12.958  16.271  89.687  1.00 43.25           O
ANISOU 2671  O   HOH   275    5298   5959   5177    -38    -58     56       O
HETATM 2672  O   HOH   276      11.965  39.155  72.079  1.00 50.64           O
ANISOU 2672  O   HOH   276    6286   6367   6587    112   -100     64       O
HETATM 2673  O   HOH   277       9.049  30.831  62.655  1.00 47.51           O
ANISOU 2673  O   HOH   277    6061   6117   5874    153      5    102       O
HETATM 2674  O   HOH   278       9.061   6.885  65.879  1.00 43.84           O
ANISOU 2674  O   HOH   278    5708   5580   5369     54     26     18       O
HETATM 2675  O   HOH   279       1.893  21.504  45.817  1.00 48.78           O
ANISOU 2675  O   HOH   279    6098   6288   6147      7    -27     -3       O
HETATM 2676  O   HOH   280       1.013  12.641  69.012  1.00 49.73           O
ANISOU 2676  O   HOH   280    6300   6303   6293   -126    -43   -107       O
HETATM 2677  O   HOH   281      14.132  37.787  79.490  1.00 49.34           O
ANISOU 2677  O   HOH   281    6249   6187   6310    -48    -42    -24       O
HETATM 2678  O   HOH   282       7.234   0.526  73.102  1.00 51.30           O
ANISOU 2678  O   HOH   282    6480   6538   6475    -60     31    -25       O
HETATM 2679  O   HOH   283      22.529  36.575  90.833  1.00 47.07           O
ANISOU 2679  O   HOH   283    6104   5905   5876     48    110    -60       O
HETATM 2680  O   HOH   286       6.203   3.972  71.037  1.00 52.76           O
ANISOU 2680  O   HOH   286    6773   6651   6623    -66    -34     43       O
HETATM 2681  O   HOH   289      -0.581   5.056  73.095  1.00 50.24           O
ANISOU 2681  O   HOH   289    6408   6252   6429   -101     43     -4       O
HETATM 2682  O   HOH   291      -0.277  21.778  87.867  1.00 37.37           O
ANISOU 2682  O   HOH   291    4444   4901   4852    104     38     69       O
HETATM 2683  O   HOH   292      41.325  35.485  71.099  1.00 49.29           O
ANISOU 2683  O   HOH   292    6371   6092   6266    -77    -46    -19       O
HETATM 2684  O   HOH   293      22.034  25.987  94.557  1.00 51.03           O
ANISOU 2684  O   HOH   293    6425   6680   6286     29      7     63       O
HETATM 2685  O   HOH   296      13.954  18.398  88.090  1.00 61.76           O
ANISOU 2685  O   HOH   296    7894   7807   7766    -32     -1      7       O
HETATM 2686  O   HOH   297       5.168  21.726  59.978  1.00 59.61           O
ANISOU 2686  O   HOH   297    7643   7504   7501     22    -82     51       O
HETATM 2687  O   HOH   298      26.854  21.908  50.588  1.00 61.24           O
ANISOU 2687  O   HOH   298    7736   7772   7759     80     49    -68       O
HETATM 2688  O   HOH   299      27.672  38.514  93.272  1.00 49.59           O
ANISOU 2688  O   HOH   299    6503   6079   6259      5      4    -47       O
HETATM 2689  O   HOH   301      21.230  36.993  82.820  1.00 47.70           O
ANISOU 2689  O   HOH   301    6164   5938   6023     54    134     -6       O
HETATM 2690  O   HOH   302      15.478  14.274  42.122  1.00 43.47           O
ANISOU 2690  O   HOH   302    5474   5495   5548     66     18    -21       O
HETATM 2691  O   HOH   303      -5.338  15.977  71.954  1.00 60.72           O
ANISOU 2691  O   HOH   303    7619   7722   7728     -3     -6     49       O
HETATM 2692  O   HOH   304      42.752  16.703  75.054  1.00 48.53           O
ANISOU 2692  O   HOH   304    6214   6081   6144    106    -20    -78       O
HETATM 2693  O   HOH   305      23.884  14.130  69.347  1.00 48.88           O
ANISOU 2693  O   HOH   305    6421   5890   6261     43   -144    -18       O
HETATM 2694  O   HOH   306      12.506  36.009  89.034  1.00 47.42           O
ANISOU 2694  O   HOH   306    5895   5874   6249    -27     41    -55       O
HETATM 2695  O   HOH   307      25.553  43.200  77.760  1.00 57.49           O
ANISOU 2695  O   HOH   307    7410   7119   7314     63     91      7       O
HETATM 2696  O   HOH   308      25.024  31.642  61.021  1.00 47.12           O
ANISOU 2696  O   HOH   308    5903   6069   5933     67     50     51       O
HETATM 2697  O   HOH   309      18.987  13.289  90.654  1.00 56.32           O
ANISOU 2697  O   HOH   309    7081   7156   7162    -43     33    -52       O
HETATM 2698  O   HOH   311      12.450  34.857  60.508  1.00 47.50           O
ANISOU 2698  O   HOH   311    6100   6005   5941    -22    -64    -27       O
HETATM 2699  O   HOH   313       6.929  37.243  50.936  1.00 53.63           O
ANISOU 2699  O   HOH   313    6873   6781   6723     -7      5     50       O
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HETATM 2700  O   HOH   314      33.831  42.307  68.854  1.00 53.16           O
ANISOU 2700  O   HOH   314    6806   6825   6567     92      7    -31       O
HETATM 2701  O   HOH   315      34.967  27.827  55.837  1.00 56.21           O
ANISOU 2701  O   HOH   315    7214   7170   6972    -42    114    -22       O
HETATM 2702  O   HOH   317      19.424  25.271  42.768  1.00 42.58           O
ANISOU 2702  O   HOH   317    5366   5677   5137     74    -53     53       O
HETATM 2703  O   HOH   318      40.816  32.777  78.372  1.00 46.80           O
ANISOU 2703  O   HOH   318    6113   5558   6113   -105      7     -5       O
HETATM 2704  O   HOH   319       2.161  14.590  46.878  1.00 59.54           O
ANISOU 2704  O   HOH   319    7579   7458   7584    -25    -34    -65       O
HETATM 2705  O   HOH   321       3.078  17.075  42.925  1.00 62.62           O
ANISOU 2705  O   HOH   321    7933   7873   7985    -12     38    -32       O
HETATM 2706  O   HOH   322       4.695  27.583  93.438  1.00 67.19           O
ANISOU 2706  O   HOH   322    8512   8561   8457    -20     23     17       O
HETATM 2707  O   HOH   323       6.865  14.509  55.845  1.00 56.89           O
ANISOU 2707  O   HOH   323    7303   7201   7110    -18      3    -10       O
HETATM 2708  O   HOH   324      15.415   4.434  85.045  1.00 55.66           O
ANISOU 2708  O   HOH   324    7140   7025   6984     63    -43     21       O
HETATM 2709  O   HOH   326      16.129   6.582  72.587  1.00 49.49           O
ANISOU 2709  O   HOH   326    6188   6233   6383    168      0    -78       O
HETATM 2710  O   HOH   327      33.441  36.723  62.911  1.00 55.80           O
ANISOU 2710  O   HOH   327    7211   7012   6980    -43      8     61       O
HETATM 2711  O   HOH   330      -0.292  24.854  78.344  1.00 56.12           O
ANISOU 2711  O   HOH   330    7181   7159   6983     58    -61     63       O
HETATM 2712  O   HOH   331      -2.262  16.030  67.431  1.00 43.84           O
ANISOU 2712  O   HOH   331    5600   5401   5657    -48   -107   -143       O
HETATM 2713  O   HOH   332       3.329  33.043  78.532  1.00 49.89           O
ANISOU 2713  O   HOH   332    6511   6227   6216     58     99    -24       O
HETATM 2714  O   HOH   335      15.236  11.644  43.279  1.00 45.72           O
ANISOU 2714  O   HOH   335    5693   5772   5905     95     33    -36       O
HETATM 2715  O   HOH   336       5.226  24.476  44.257  1.00 46.11           O
ANISOU 2715  O   HOH   336    5835   6003   5682     -2     47     52       O
HETATM 2716  O   HOH   338      37.716  19.152  63.872  1.00 47.85           O
ANISOU 2716  O   HOH   338    6149   5815   6217    -10     83    -36       O
HETATM 2717  O   HOH   340      -0.279  14.811  65.962  1.00 55.82           O
ANISOU 2717  O   HOH   340    7087   7100   7020     49    -30    -30       O
HETATM 2718  O   HOH   341      17.272  10.150  42.135  1.00 46.09           O
ANISOU 2718  O   HOH   341    5845   5850   5817   -109     -6      3       O
HETATM 2719  O   HOH   342      33.731  21.964  59.151  1.00 48.16           O
ANISOU 2719  O   HOH   342    6050   6261   5987    -82     99   -143       O
HETATM 2720  O   HOH   343       3.315  13.263  67.070  1.00 54.80           O
ANISOU 2720  O   HOH   343    6862   6874   7087    -87     87    -19       O
HETATM 2721  O   HOH   344       9.552  29.955  43.445  1.00 47.43           O
ANISOU 2721  O   HOH   344    6003   5977   6040     39    -96     -3       O
HETATM 2722  O   HOH   345      31.518  37.945  65.887  1.00 47.47           O
ANISOU 2722  O   HOH   345    6008   5995   6035    -80    135     28       O
HETATM 2723  O   HOH   347      11.233   7.838  64.305  1.00 53.52           O
ANISOU 2723  O   HOH   347    6849   6681   6806     53    -13   -110       O
HETATM 2724  O   HOH   350      13.328  38.241  87.887  1.00 47.64           O
ANISOU 2724  O   HOH   350    5962   5927   6213   -116     46    -19       O
HETATM 2725  O   HOH   351      25.523  36.758  93.170  1.00 60.03           O
ANISOU 2725  O   HOH   351    7656   7563   7589     -5     13     29       O
HETATM 2726  O   HOH   352      26.921  40.234  91.104  1.00 51.06           O
ANISOU 2726  O   HOH   352    6818   5989   6592   -117    -54     15       O
HETATM 2727  O   HOH   353      13.055   2.690  69.900  1.00 62.11           O
ANISOU 2727  O   HOH   353    7940   7809   7849     21    -46    -47       O
HETATM 2728  O   HOH   355       2.495  34.790  83.626  1.00 48.14           O
ANISOU 2728  O   HOH   355    6003   5987   6301     77   -181     11       O
HETATM 2729  O   HOH   357       8.408  13.997  61.499  1.00 47.34           O
ANISOU 2729  O   HOH   357    6049   5853   6087    -82     27   -128       O
HETATM 2730  O   HOH   358      17.978   9.188  71.905  1.00 59.37           O
ANISOU 2730  O   HOH   358    7436   7550   7574     47    -55    -21       O
HETATM 2731  O   HOH   359      25.220  24.855  47.581  1.00 56.34           O
ANISOU 2731  O   HOH   359    7003   7178   7226    -35     49     48       O
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HETATM 2732  O   HOH   360       8.365  39.797  52.554  1.00 57.70           O
ANISOU 2732  O   HOH   360     7369   7257   7299     24     14     30       O
HETATM 2733  O   HOH   362       8.453   6.194  85.366  1.00 43.29           O
ANISOU 2733  O   HOH   362     5448   5321   5681   -170     22     39       O
HETATM 2734  O   HOH   364       3.892  23.307  62.053  1.00 52.89           O
ANISOU 2734  O   HOH   364     6740   6637   6718     13    -39     -1       O
HETATM 2735  O   HOH   365      22.092  41.480  85.519  1.00 59.49           O
ANISOU 2735  O   HOH   365     7576   7466   7560    -20     -9    -41       O
HETATM 2736  O   HOH   366      14.864  41.955  74.200  1.00 52.35           O
ANISOU 2736  O   HOH   366     6698   6451   6742     35      3      6       O
HETATM 2737  O   HOH   367       3.269  23.566  51.675  1.00 54.55           O
ANISOU 2737  O   HOH   367     6765   6914   7048     39    -82    -15       O
HETATM 2738  O   HOH   369       7.946   3.294  79.018  1.00 48.66           O
ANISOU 2738  O   HOH   369     6277   5968   6242    -38     46     23       O
HETATM 2739  O   HOH   371      -5.312   7.469  77.838  1.00 56.64           O
ANISOU 2739  O   HOH   371     7159   7120   7242    -88    -16     44       O
HETATM 2740  O   HOH   372      12.502  34.453  69.116  1.00 50.93           O
ANISOU 2740  O   HOH   372     6395   6446   6509     39    -96    -23       O
HETATM 2741  O   HOH   373      23.748  29.185  56.362  1.00 51.90           O
ANISOU 2741  O   HOH   373     6496   6645   6580     42     77     20       O
HETATM 2742  O   HOH   374      25.326  36.263  68.141  1.00 45.43           O
ANISOU 2742  O   HOH   374     5757   5923   5580     50     35    159       O
HETATM 2743  O   HOH   375       4.034  36.060  89.188  1.00 52.68           O
ANISOU 2743  O   HOH   375     6664   6524   6830    108     32   -119       O
HETATM 2744  O   HOH   376       8.774  37.413  89.385  1.00 58.93           O
ANISOU 2744  O   HOH   376     7501   7465   7425    -42     34    -78       O
HETATM 2745  O   HOH   377      39.698  40.850  59.792  1.00 56.29           O
ANISOU 2745  O   HOH   377     7140   7108   7139    -63     16    -48       O
HETATM 2746  O   HOH   378      13.215  24.355  40.367  1.00 49.52           O
ANISOU 2746  O   HOH   378     6422   6371   6024    -84     96    147       O
HETATM 2747  O   HOH   380      20.951  39.755  83.302  1.00 54.05           O
ANISOU 2747  O   HOH   380     6742   6918   6877      8    -16     36       O
HETATM 2748  O   HOH   381      16.135  12.472  61.601  1.00 56.44           O
ANISOU 2748  O   HOH   381     7190   7125   7131      7     55    -11       O
HETATM 2749  O   HOH   382      21.722  14.220  67.972  1.00 63.83           O
ANISOU 2749  O   HOH   382     8090   8138   8024    -41    -10     16       O
HETATM 2750  O   HOH   384       6.011  11.185  67.542  1.00 57.41           O
ANISOU 2750  O   HOH   384     7324   7183   7305     45     -5     86       O
HETATM 2751  O   HOH   385      17.439  40.675  87.096  1.00 58.27           O
ANISOU 2751  O   HOH   385     7270   7407   7463    107     29    -36       O
HETATM 2752  O   HOH   386      45.716  33.327  69.519  1.00 49.83           O
ANISOU 2752  O   HOH   386     6362   6243   6329   -120      2    -24       O
HETATM 2753  O   HOH   394      14.879   4.605  70.173  1.00 55.59           O
ANISOU 2753  O   HOH   394     7098   6966   7058     28    -55     68       O
HETATM 2754  O   HOH   396       9.997  11.781  91.683  1.00 57.00           O
ANISOU 2754  O   HOH   396     6965   7380   7314    -10     -7    -10       O
HETATM 2755  O   HOH   398       0.496  16.727  50.862  1.00 58.43           O
ANISOU 2755  O   HOH   398     7313   7415   7474    -20     -5    -24       O
HETATM 2756  O   HOH   399       2.187  20.776  54.264  1.00 51.45           O
ANISOU 2756  O   HOH   399     6482   6690   6376    -10     91   -100       O
HETATM 2757  O   HOH   400      31.245  20.318  56.035  1.00 54.12           O
ANISOU 2757  O   HOH   400     6761   7015   6787    -19    -21    -87       O
HETATM 2758  O   HOH   401       3.637  13.527  60.726  1.00 64.33           O
ANISOU 2758  O   HOH   401     8139   8215   8087    -60    -19     -6       O
HETATM 2759  O   HOH   403       3.546   4.378  70.862  1.00 61.55           O
ANISOU 2759  O   HOH   403     7951   7653   7782    -64     16    -30       O
HETATM 2760  O   HOH   413      41.302  18.266  82.469  1.00 51.62           O
ANISOU 2760  O   HOH   413     6539   6611   6463     67   -113    -36       O
HETATM 2761  O   HOH   414      37.305  36.992  70.772  1.00 55.58           O
ANISOU 2761  O   HOH   414     7055   7074   6990    -12     73     29       O
HETATM 2762  O   HOH   416      -0.907  21.900  85.346  1.00 41.86           O
ANISOU 2762  O   HOH   416     5163   5398   5342     49     72      5       O
HETATM 2763  O   HOH   417       6.864  32.422  79.415  1.00 52.77           O
ANISOU 2763  O   HOH   417     6687   6550   6815    172     -1     17       O
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HETATM 2764  O   HOH   418       7.481  39.091  75.571  1.00 59.45           O
ANISOU 2764  O   HOH   418    7482   7522   7584      0      0    -13       O
HETATM 2765  O   HOH   419      27.524  39.365  73.684  1.00 25.45           O
ANISOU 2765  O   HOH   419    2857   3298   3514   -125    281    584       O
HETATM 2766  O   HOH   420      -0.025  28.677  90.592  1.00 65.13           O
ANISOU 2766  O   HOH   420    8228   8291   8227    -27     90    -41       O
HETATM 2767  O   HOH   425      40.888  16.331  73.180  1.00 61.78           O
ANISOU 2767  O   HOH   425    7832   7717   7926      9     -4     26       O
HETATM 2768  O   HOH   426      28.444  41.518  73.525  1.00 37.04           O
ANISOU 2768  O   HOH   426    4734   4158   5182    -53     20    -25       O
HETATM 2769  O   HOH   427      16.016   3.824  82.316  1.00 57.82           O
ANISOU 2769  O   HOH   427    7247   7319   7403    -26    -41     16       O
HETATM 2770  O   HOH   428      23.420  41.821  73.723  1.00 45.39           O
ANISOU 2770  O   HOH   428    5489   5889   5866    -26     -7    109       O
HETATM 2771  O   HOH   429      12.812   4.190  66.701  1.00 59.20           O
ANISOU 2771  O   HOH   429    7463   7442   7588    -30     30      2       O
HETATM 2772  O   HOH   430       6.360  35.019  76.713  1.00 59.09           O
ANISOU 2772  O   HOH   430    7361   7558   7532    -11      1    -48       O
HETATM 2773  O   HOH   432       4.119  32.067  92.209  1.00 51.99           O
ANISOU 2773  O   HOH   432    6557   6663   6534      4     80    -80       O
HETATM 2774  O   HOH   437       6.623  12.969  48.482  1.00 56.87           O
ANISOU 2774  O   HOH   437    7364   7116   7127     44     -1    -48       O
HETATM 2775  O   HOH   440      12.750  40.608  70.163  1.00 55.18           O
ANISOU 2775  O   HOH   440    6954   6998   7015     28     47    -23       O
HETATM 2776  O   HOH   441       7.126   2.530  67.794  1.00 59.18           O
ANISOU 2776  O   HOH   441    7546   7460   7480    -61    -36    -48       O
HETATM 2777  O   HOH   443      46.670  25.492  68.517  1.00 61.08           O
ANISOU 2777  O   HOH   443    7683   7754   7769     27     72     13       O
HETATM 2778  O   HOH   445       6.871  30.879  95.965  1.00 55.71           O
ANISOU 2778  O   HOH   445    7018   7146   7002     12    -10     46       O
HETATM 2779  O   HOH   451      15.622  12.679  58.773  1.00 61.40           O
ANISOU 2779  O   HOH   451    7791   7823   7716      9    -88    -11       O
HETATM 2780  O   HOH   452      25.689  28.519  54.413  1.00 62.21           O
ANISOU 2780  O   HOH   452    7785   7966   7887    -41     14     26       O
HETATM 2781  O   HOH   457      41.314  16.986  88.613  1.00 48.52           O
ANISOU 2781  O   HOH   457    6011   6194   6231     92      5     47       O
HETATM 2782  O   HOH   465      24.829  40.922  69.886  1.00 44.56           O
ANISOU 2782  O   HOH   465    5771   5485   5673     12     15     34       O
HETATM 2783  O   HOH   467       6.762  36.046  61.809  1.00 56.72           O
ANISOU 2783  O   HOH   467    7186   7159   7205      4      3      8       O
HETATM 2784  O   HOH   472      11.158  39.890  87.944  1.00 57.13           O
ANISOU 2784  O   HOH   472    7284   7170   7253     -3     28     31       O
HETATM 2785  O   HOH   473      31.538  12.268  75.175  1.00 51.92           O
ANISOU 2785  O   HOH   473    6705   6525   6496    -25     51    -14       O
HETATM 2786  O   HOH   476      26.979  13.822  60.648  1.00 42.36           O
ANISOU 2786  O   HOH   476    5511   5199   5384      9    105      7       O
HETATM 2787  O   HOH   477      21.273  37.456  63.586  1.00 54.55           O
ANISOU 2787  O   HOH   477    6835   6933   6957    -34     40     48       O
HETATM 2788  O   HOH   481      20.412  35.837  50.187  1.00 51.97           O
ANISOU 2788  O   HOH   481    6452   6741   6555    -93     48      2       O
HETATM 2789  O   HOH   482      39.521  42.897  65.639  1.00 58.39           O
ANISOU 2789  O   HOH   482    7504   7396   7285    -33     69     -7       O
HETATM 2790  O   HOH   483      24.823   8.540  69.442  1.00 59.90           O
ANISOU 2790  O   HOH   483    7700   7472   7588    -65     -2      3       O
HETATM 2791  O   HOH   487       5.944  34.999  92.476  1.00 56.11           O
ANISOU 2791  O   HOH   487    7054   7203   7062    -16     42    -19       O
HETATM 2792  O   HOH   488      37.642  14.987  63.395  1.00 47.50           O
ANISOU 2792  O   HOH   488    5941   5990   6117     98    102    -11       O
HETATM 2793  O   HOH   489      41.015  38.881  64.470  1.00 55.54           O
ANISOU 2793  O   HOH   489    7016   6923   7165     -8     23    -31       O
HETATM 2794  O   HOH   491      32.734  18.593  58.165  1.00 53.69           O
ANISOU 2794  O   HOH   491    6728   6899   6773     47    -24    -98       O
HETATM 2795  O   HOH   493       8.740   7.839  89.511  1.00 58.03           O
ANISOU 2795  O   HOH   493    7350   7327   7372    -11    -45     70       O
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HETATM 2796  O   HOH   495      23.604  25.929  44.812  1.00 56.41           O
ANISOU 2796  O   HOH   495    7030   7253   7153     98     63    -21       O
HETATM 2797  O   HOH   500       0.474  27.705  86.600  1.00 48.77           O
ANISOU 2797  O   HOH   500    6246   6507   5777    331   -175   -101       O
HETATM 2798  O   HOH   504      25.631  32.751  48.064  1.00 65.67           O
ANISOU 2798  O   HOH   504    8285   8326   8342     -8     25     18       O
HETATM 2799  O   HOH   506      19.513   4.664  81.284  1.00 62.16           O
ANISOU 2799  O   HOH   506    7807   7850   7961     -7    -67    -14       O
HETATM 2800  O   HOH   509      21.454  17.148  40.997  1.00 56.69           O
ANISOU 2800  O   HOH   509    6992   7285   7262     26    -33      3       O
HETATM 2801  O   HOH   514      18.388  40.807  69.422  1.00 59.00           O
ANISOU 2801  O   HOH   514    7435   7516   7467      9    -10     19       O
HETATM 2802  O   HOH   515       8.190  38.470  57.852  1.00 59.17           O
ANISOU 2802  O   HOH   515    7415   7446   7622     -3    -72     88       O
HETATM 2803  O   HOH   517      43.777  32.298  64.059  1.00 61.31           O
ANISOU 2803  O   HOH   517    7705   7778   7813    -33     72     75       O
HETATM 2804  O   HOH   519      25.135  36.655  71.139  1.00 50.29           O
ANISOU 2804  O   HOH   519    6713   6286   6111    241     -9     45       O
HETATM 2805  O   HOH   522      16.923   7.483  41.655  1.00 52.27           O
ANISOU 2805  O   HOH   522    6598   6563   6700    -41     48    -17       O
HETATM 2806  O   HOH   523      11.324   2.417  78.141  1.00 62.13           O
ANISOU 2806  O   HOH   523    7828   7925   7853     21     21     50       O
HETATM 2807  O   HOH   526      33.616  13.704  92.622  1.00 52.56           O
ANISOU 2807  O   HOH   526    6856   6504   6609      2    -19     32       O
HETATM 2808  O   HOH   530      40.594  19.720  85.115  1.00 59.54           O
ANISOU 2808  O   HOH   530    7343   7643   7637      6    -50      2       O
HETATM 2809  O   HOH   532      15.076  31.487  94.187  1.00 54.80           O
ANISOU 2809  O   HOH   532    6794   7049   6979    -22     16      3       O
HETATM 2810  O   HOH   533      29.531  25.159  95.169  1.00 60.30           O
ANISOU 2810  O   HOH   533    7650   7631   7631    -35    -35     34       O
HETATM 2811  O   HOH   537      28.865  20.427  53.190  1.00 61.62           O
ANISOU 2811  O   HOH   537    7694   7884   7833      7     63      7       O
HETATM 2812  O   HOH   540       3.488  19.765  56.474  1.00 55.51           O
ANISOU 2812  O   HOH   540    6849   7169   7075     77      1     13       O
HETATM 2813  O   HOH   544       1.976  26.521  93.596  1.00 55.30           O
ANISOU 2813  O   HOH   544    6950   7025   7035     50     74     42       O
HETATM 2814  O   HOH   545       6.232  26.717  42.963  1.00 61.67           O
ANISOU 2814  O   HOH   545    7843   7854   7736     41    -36    -18       O
HETATM 2815  O   HOH   547      15.978  43.004  78.376  1.00 54.93           O
ANISOU 2815  O   HOH   547    6775   6976   7120     29    -47    -37       O
HETATM 2816  O   HOH   552      23.478  11.461  69.512  1.00 48.39           O
ANISOU 2816  O   HOH   552    6368   5943   6074     34     34    -38       O
HETATM 2817  O   HOH   564      31.768  13.802  72.785  1.00 50.67           O
ANISOU 2817  O   HOH   564    6430   6380   6444     37    -36    -82       O
HETATM 2818  O   HOH   565      43.097  17.088  70.385  1.00 48.92           O
ANISOU 2818  O   HOH   565    6012   6253   6323    209     41    -81       O
HETATM 2819  O   HOH   578      25.824  12.068  89.747  1.00 49.43           O
ANISOU 2819  O   HOH   578    6241   6143   6397    115     23     18       O
HETATM 2820  O   HOH   579      13.391  34.227  97.272  1.00 63.68           O
ANISOU 2820  O   HOH   579    8088   8000   8106    -32      0    -28       O
HETATM 2821  O   HOH   583      16.532  18.164  87.980  1.00 51.16           O
ANISOU 2821  O   HOH   583    6539   6406   6493    -38     73    105       O
HETATM 2822  O   HOH   591      24.443  15.964  52.058  1.00 50.29           O
ANISOU 2822  O   HOH   591    6313   6394   6401     -2     10      8       O
HETATM 2823  O   HOH   592      11.355  36.376  65.514  1.00 52.43           O
ANISOU 2823  O   HOH   592    6660   6474   6786     67    -21      4       O
HETATM 2824  O   HOH   593      37.256  22.800  90.212  1.00 43.47           O
ANISOU 2824  O   HOH   593    5247   5701   5566    -27    -83    130       O
HETATM 2825  O   HOH   600      18.701   9.992  44.274  1.00 55.16           O
ANISOU 2825  O   HOH   600    6999   7033   6926     47     14   -113       O
HETATM 2826  O   HOH   615      25.210  19.141  47.805  1.00 57.78           O
ANISOU 2826  O   HOH   615    7249   7324   7380     79     76     19       O
HETATM 2827  O   HOH   616      22.084  11.729  51.994  1.00 58.99           O
ANISOU 2827  O   HOH   616    7480   7441   7493     60      2    -88       O
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HETATM 2828  O   HOH   619      41.178  27.721  77.339  1.00 37.71           O
ANISOU 2828  O   HOH   619    4854   4339   5135    298   -117   -214       O
HETATM 2829  O   HOH   623      -1.197  26.206  72.921  1.00 53.43           O
ANISOU 2829  O   HOH   623    6708   6883   6709    -27      2     75       O
HETATM 2830  O   HOH   624      45.484  20.006  82.208  1.00 56.64           O
ANISOU 2830  O   HOH   624    7255   7139   7127    -13     -7     17       O
HETATM 2831  O   HOH   627      11.143  -2.160  66.228  1.00 62.12           O
ANISOU 2831  O   HOH   627    7798   7880   7927    -33    -16     27       O
HETATM 2832  O   HOH   637      19.352  15.446  62.934  1.00 45.54           O
ANISOU 2832  O   HOH   637    5887   5559   5855    -40    -83   -140       O
HETATM 2833  O   HOH   640      -2.217   4.066  79.725  1.00 60.76           O
ANISOU 2833  O   HOH   640    7688   7739   7658    -42      5     28       O
HETATM 2834  O   HOH   657      10.956  43.002  53.601  1.00 48.01           O
ANISOU 2834  O   HOH   657    6210   5918   6113     93      1     -9       O
HETATM 2835  O   HOH   658      47.384  16.959  79.217  1.00 61.75           O
ANISOU 2835  O   HOH   658    7871   7747   7846     39    -30     17       O
HETATM 2836  O   HOH   663      11.745  36.372  72.089  1.00 61.47           O
ANISOU 2836  O   HOH   663    7726   7864   7766     23    -58     11       O
HETATM 2837  O   HOH   667       2.304  27.310  61.929  1.00 49.79           O
ANISOU 2837  O   HOH   667    6160   6349   6410      3    -16    125       O
HETATM 2838  O   HOH   669      23.828  39.012  67.662  1.00 52.84           O
ANISOU 2838  O   HOH   669    6570   6660   6846   -100     56    -17       O
HETATM 2839  O   HOH   673      11.087  47.504  65.109  1.00 62.37           O
ANISOU 2839  O   HOH   673    7841   7952   7907    -26     11    -13       O
HETATM 2840  O   HOH   676      14.238  10.438  50.818  1.00 62.35           O
ANISOU 2840  O   HOH   676    7984   7857   7850      9     20    -25       O
HETATM 2841  O   HOH   681      31.791  26.751  94.935  1.00 47.57           O
ANISOU 2841  O   HOH   681    6146   6031   5899    -95   -168    134       O
HETATM 2842  O   HOH   684      37.979  38.970  68.454  1.00 53.13           O
ANISOU 2842  O   HOH   684    6769   6666   6752   -117    121    -38       O
HETATM 2843  O   HOH   699      41.716  19.258  67.307  1.00 57.26           O
ANISOU 2843  O   HOH   699    7261   7338   7158     60     23      2       O
HETATM 2844  O   HOH   703      21.774   9.807  71.073  1.00 58.05           O
ANISOU 2844  O   HOH   703    7354   7235   7467    -65    -23     -4       O
HETATM 2845  O   HOH   708      17.768  41.625  80.761  1.00 57.03           O
ANISOU 2845  O   HOH   708    7218   7256   7196     62     37    -76       O
HETATM 2846  O   HOH   710       9.677  39.234  68.814  1.00 59.73           O
ANISOU 2846  O   HOH   710    7430   7620   7646     83    -10     12       O
HETATM 2847  O   HOH   713      15.316  17.548  35.927  1.00 53.94           O
ANISOU 2847  O   HOH   713    6916   6622   6956    -37     33     87       O
HETATM 2848  O   HOH   714      29.308  14.272  58.997  1.00 61.71           O
ANISOU 2848  O   HOH   714    7801   7844   7803     -2    -49    -38       O
HETATM 2849  O   HOH   718      39.719  18.245  89.381  1.00 58.93           O
ANISOU 2849  O   HOH   718    7550   7394   7446     20    -47    -26       O
HETATM 2850  O   HOH   745      40.826  15.163  70.694  1.00 62.25           O
ANISOU 2850  O   HOH   745    7927   7817   7908     40    -35     42       O
HETATM 2851  O   HOH   746      13.165  -0.800  71.540  1.00 60.38           O
ANISOU 2851  O   HOH   746    7607   7643   7692     25     29    -62       O
CONECT 1473 2417
CONECT 2417 1473
MASTER      331    0    0   13   12    0    0    6 2849    2    2   24
END
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